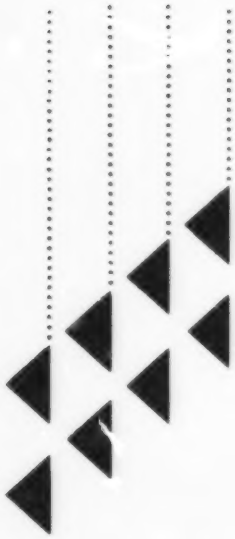
Health and Welfare Canada
Santé et Bien-être social Canada

A Survey and Critical Review of Models to Assess Human Exposure to Chemicals



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A Survey and Critical Review of Models to Assess Human Exposure to Chemicals

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Health Protection Branch

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A report for the Health Protection Branch of Health and Welfare Canada by Donald Mackay and Sally Paterson, Institute for Environmental Studies, University of Toronto.

Executive Summary

The Canadian Environmental Protection Act (CEPA) requires the assessment of chemicals that are new to Canada, based upon the set of data provided by the manufacturer or importer on their physical, chemical and toxicity properties and their intended use patterns. Part of the assessment process may use computer models to estimate the nature and extent of human exposure that will result from commercial use of these chemicals. As no models suitable for immediate implementation are available within the federal government, this report reviews models and modelling approaches in use or being developed in other jurisdictions. A search of literature and contact with key agencies elicited 15 models or modelling approaches which touch upon the assessment of human exposure to new chemicals. These models are reviewed and their strengths and deficiencies are discussed. No one existing model can be adopted immediately by Health and Welfare Canada for application under CEPA, but it should be possible to assemble a model suitable for the purposes of Health and Welfare Canada and applicable to the specific needs of Canadian conditions within one or two years by adapting various modules from existing models. A program to achieve this objective is outlined and recommendations are made for the optimal approach.

Table of Contents

		Page
1.	**Introduction**	7
1.1	General	7
1.2	Approach in this Report	11
2.	**Inventory of Models and Approaches**	12
2.1	The Search Process	12
2.2	Inventory of Models	14
	A: GEOTOX	14
	B: Remedial Action Priority System (RAPS)	17
	C: Multi-phase Non-steady State Equilibrium Model (MNSEM)	23
	D: Persistence	26
	E: Environmental Exposure Potentials (EEP)	30
	F: Environmental Partitioning Model (ENPART)	33
	G: TOXSCREEN	34
	H: Exposure Commitment Method	35
	I: Preliminary Pollutant Limit Value (PPLV)	36
	J: Fugacity Models	39
	K: SIMPLESAL	41
	L: Aid for Evaluating the Redevelopment of Industrial Sites (AERIS)	42
	M: Multimedia-Compartmental Model (MCM)	44
3.	**Critical Evaluation**	45
3.1	Summary Spreadsheet	45
3.2	Are These Models Suitable for Use Under CEPA?	48
3.3	What Type of Model is Needed?	48
3.3.1	The Nature of Models	48
3.3.2	Canadian Regulatory Considerations	49
3.3.3	Canadian Geographic Considerations	49
3.3.4	Fugacity and Concentration Models	49
3.4.	What Should Health and Welfare Canada Do?	50
4.	**Conclusions**	52
References and Bibliography		53
Appendix		55
References to Appendix		61

List of Tables

		Page
1.1	"Intermediate" Information Requirements	8
1.2	"Full" Information Requirements	9
2.1	Draft Compendium of Environmental Exposure Assessment Methods for Chemicals	12
A.1	Daily doses predicted for the seven exposure pathways after the release of 1 mol/km^2-year of each contaminant into the upper soil compartment	16
A.2	Comparison of estimated contaminant dose rates from all exposure pathways and Virtually Safe Dose Rates (VSDR)	16
C.1	Summary of environmental fate of naphthalene, evaluated by multi-phase non-steady equilibrium model (version 1.3)	25
D.1	Basic design of the persistence model	28
D.2	Predicted distribution and degradation routes of hexachlorobenzene at steady state using the persistence model and the standard pond and standard lake system parameters	28
E.1	Print-out of input-data and results	31
H.1	Current levels of lead in the background Environment and in humans	35
I.1	PPLV worksheet	38
I.2	Symbols and abbreviations involved in the Calculations	38
J.1	Calculated and reported concentrations for the four bulk phases and fish and bulk phase fugacities	40

		Page
3.1	Summary spreadsheet of the models and their characteristics	46
3.2	Summary of quantitative methods	55

List of Figures

1.1	Environmental fate processes	10
A.1	Conceptual diagram of the major compartments, phases and pathways addressed in the screening methodology	15
A.2	Schematic of the cattle/meat/dairy product pathway model	15
B.1	Simplified diagram outlining the interactions between the transport pathways and exposure assessment components of the RAPS methodology	18
B.2	Exposure pathways considered by RAPS	19
B.3	Exposure pathways to humans	20
C.1	Schematic diagram of environmental fate	24
D.1	Basic design of the persistence model	27
D.2	Accumulation of hexachlorobenzene before, during and after steady state is reached in the compartments of the standard pond and lake of the persistence model	29
E.1	Fingerprint of parameters	32
I.1	Pathways from soil via water, plant and animal compartments to humans	37
K.1	SIMPLESAL processes	42
3.1	Suggested assessment regions in Canada	51

1. Introduction

1.1 General

Canadian Environmental Protection Act, promulgated in 1988, requires Environment Canada and Health and Welfare Canada (H&W) to assess the environmental fate, effects and human exposure of chemicals that are new to Canada. In the US approximately 1000 new chemicals are submitted for assessment annually, but it is expected that in Canada the number will be smaller, perhaps 100 to 200 per year. Canada-US comparisons can, however, be misleading because of differences in notification requirements and notifiable quantities. It will be necessary to develop a well-defined, scientifically rigorous and generally acceptable procedure by which the available input data on chemical properties and toxicity are processed to arrive at an assessment of human exposure and ultimately risk. Ideally, this procedure should be readily available so that those planning to market a specific chemical can determine in advance the likely response of the regulating agency. An attractive option is to use one or more computer models to conduct this assessment since models minimize the element of personal judgement, reduce the probability of human error in the assessment process and give rapid and repeatable output.

The preferred approach is to use mechanistic models, in which the input data are used to calculate the environmental partitioning tendencies of the chemicals, resulting in estimated concentrations in compartments such as air, water, soil, fish, sediment, and vegetation. From these concentrations the presence of chemicals in human exposure media (air, water and foodstuffs) can be calculated and total dosages to humans calculated in units, for example, of micrograms per day. It is also possible to link these models to pharmacokinetic models describing the fate of the chemical within the human body so that concentrations of chemical in target tissues can be estimated. This report focuses primarily on models of this general type, which can vary greatly in complexity, in geographical area of application, and in the emphasis on various human exposure routes. A second approach is to use scoring systems in which input data are converted into scoring points reflecting a perceived level of concern, which are combined to give an overall score representing the severity of exposure or the effect. An example of this approach is the Ontario vector system, which is used to establish the list of priority pollutants in that province. Although such systems are easier to use and understand, they fail to give a quantitative estimation of human exposure. They do not identify specific routes of exposure, and in certain cases they may give misleading results. They are primarily of use in establishing lists of priority chemicals, and for screening those which deserve further study. Such models are considered only briefly in this report.

The chemical property information required under CEPA varies depending on whether or not the substance is specified on the "Domestic" or the "Non-domestic" Substances List, and the quantity of the substance to be manufactured or imported each year. These lists are presently being compiled by Environment Canada. Three levels of information requirement have been established, basic, intermediate and full. Only the intermediate and full requirements are relevant to this report; three are specified in Tables 1.1 and 1.2. The essential task of a model is to use data obtained from these requirements to calculate environmental partitioning characteristics, concentrations in the media of human exposure and tissue concentrations in humans exposed to these chemicals. Figure 1.1 is an illustration of the nature of some of the more important environmental human exposure pathways. The model can be regarded as a tool for estimating the quantity and concentration of chemical that will reside in media illustrated in Figure 1.1 and the quantities that flow along the various pathways towards a typical human receptor.

Table 1.1
"Intermediate" Information Requirements

1. (a) The chemical name of the substance, established in accordance with the chemical nomenclature rules of the International Union of Pure and Applied Chemistry or the Chemical Abstract Service.

   (b) Trade names or synonyms of the chemical name, if known.

   (c) Chemical Abstracts Service registry number for the substance, if such a number can be assigned.

   (d) Structural formula and gram molecular weight of the substance; degree of purity of technical grade product if applicable; known impurities and their concentration by weight; and additives and stabilizers essential for the purposes of marketing, and their concentrations by weight.

   (e) The material safety data sheet, as defined in the *Hazardous Products Act*, for the substance, if available.

2. (a) The following physical and chemical data: melting point; boiling point; density; vapour pressure; water solubility; octanol-water partition coefficient; infrared; ultra-violet; mass or nuclear magnetic resonance spectra suitable for characterization of the substance; dissociation constant; adsorption and desorption screening test data; hydrolysis as a function of pH and if known, identification of the products of hydrolysis; and particle size or fibre length distribution data, if applicable.

   (b) Test data from one acute mammalian oral, dermal or inhalation toxicity test, representing the most significant route of potential human exposure to the substance.

   (c) Age, sex, number, species, strain and source of animals tested; route and conditions of administration; and dose, concentration and vehicle of test substances for the test referred to in sub-item 2(2).

   (d) All other information and test data relevant to environmental and health hazard identification that is in the person's possession or to which the person ought reasonably to have access.

   (e) Description or specification of laboratory procedures followed in developing test data, including, for data developed after these regulations come into force or for test procedures that are not prescribed, test methods, reference substances and quality control and quality assurance procedures.

3. (a) Manufacture, importation, use and disposal information, including estimated annual manufacture and importation rates, intended uses, and recommended handling, transport, storage, destruction or disposal methods for the substance.

   (b) Anticipated nature and extent of emissions and discharges of the substance to the environment.

   (c) Estimated number of persons, if known, that may become exposed to the substance.

4. Identification of other government agencies, either foreign or within Canada, that have been notified of the manufacture or importation of the substance, and the purpose of such notification.

Table 1.2
"Full" Information Requirements.

1. (a) The chemical name of the substance, established in accordance with the chemical nomenclature rules of the International Union of Pure and Applied Chemistry or the Chemical Abstract Service.

   (b) Chemical Abstracts Service registry number for the substance, if such a number can be assigned.

   (c) Structural formula; degree of purity of technical grade product if applicable; known impurities and their concentration by weight; and additives and stabilizers essential for the purposes of marketing, and their concentrations by weight.

   (d) The material safety data sheet, as defined in the *Hazardous Products Act*, for the substance, if available.

2. (a) The following physical and chemical data: melting point; boiling point; density; vapour pressure; water solubility; octanol-water partition coefficient; infrared; ultra-violet; mass or nuclear magnetic resonance spectra suitable for characterization of the substance; dissociation constant; adsorption and desorption screening test data; hydrolysis as a function of pH and if known, identification of the products of hydrolysis; and particle size or fibre length distribution data, if applicable.

   (b) Test data from two acute mammalian toxicity tests, representing the two most significant of oral, dermal or inhalation routes of potential human exposure to the substance.

   (c) Test data from one skin irritation test and one skin sensitization test.

   (d) Repeated dose mammalian toxicity test data from one test of at least 14 days duration (28 days preferred) representing the most significant route of potential human exposure.

   (e) Age, sex, number, species, strain and source of animals tested, route and conditions of administration, and dose, concentration and vehicle of test substances for tests referred to in sub-items (2), (3) and (4).

   (f) Mutagenicity test data obtained from the following tests:

   - one *in vitro* test, with and without metabolic activation, for gene mutations;

   - one *in vitro* test, with and without metabolic activation, for chromosomal aberrations in mammalian cells;

   - one *in vivo* test for chromosomal aberrations demonstrating exposure of the tissue tested, to the substance or its metabolites at sufficient concentrations; and

   - one *in vivo* mammalian test for chromosomal aberrations, gene mutations, or other acceptable endpoint in another tissue demonstrating exposure of the substance or its metabolites at sufficient concentrations.

   (g) Fish and daphnia acute toxicity test data, including limit test or LC_{50} results as appropriate.

   (h) Ready biodegradability test data and if known, identification of the products of biodegradation.

   (i) Bioaccumulation test data (sequential static fish test, semi-static fish test, degree of bioconcentration in fish test or flow through fish test data only).

   (j) All other information and test data relevant to environmental and health hazard identification that is in the person's possession or to which the person ought reasonably to have access.

   (k) Description or specification of laboratory procedures followed in developing test data, including, for data developed after these regulations come into force or for test procedures that are not prescribed, test methods, reference substances and quality control and quality assurance procedures.

3. (a) Manufacture, importation, use and disposal information, including estimated annual manufacture and importation rates, intended uses, and recommended handling, transport, storage, destruction or disposal methods for the substance.

   (b) Recommended precautions and emergency measures, including personal protective equipment, engineering controls, leak and spill clean-up procedures, handling procedures, storage requirements, and first aid measures.

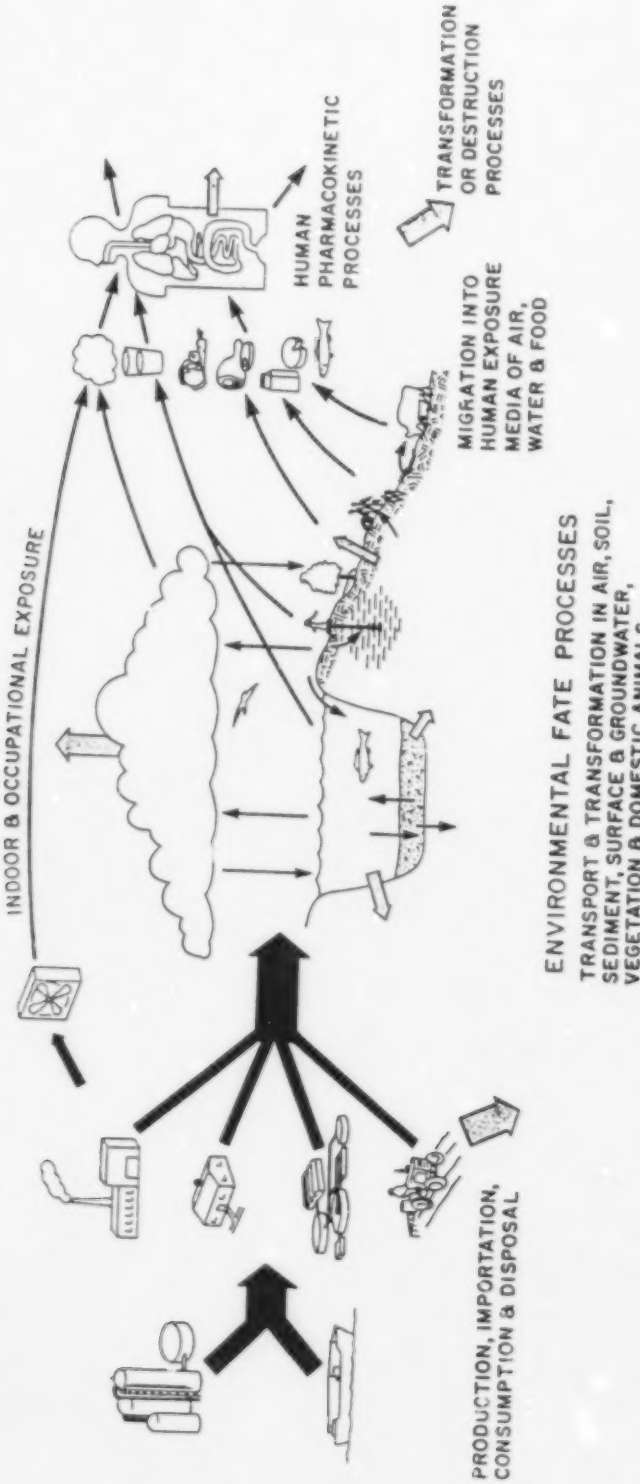
   (c) Anticipated nature and extent of emissions and discharges of the substance to the environment.

   (d) Estimated number of persons, if known, that may become exposed to the substance.

4. Full descriptions of or specifications to analytical methods that can be used for detection and determination of concentrations of the substance at or below the LC_{50} levels reported in sub-item 2(7).

5. Identification of other government agencies, either foreign or within Canada, that the person has notified of the manufacture or importation of the substance, and the purpose of such notification.

Figure 1.1
Environmental fate processes


INDOOR & OCCUPATIONAL EXPOSURE
HUMAN PHARMACOKINETIC PROCESSES
TRANSFORMATION OR DESTRUCTION PROCESSES
MIGRATION INTO HUMAN EXPOSURE MEDIA OF AIR, WATER & FOOD
ENVIRONMENTAL FATE PROCESSES
TRANSPORT & TRANSFORMATION IN AIR, SOIL, SEDIMENT, SURFACE & GROUNDWATER, VEGETATION & DOMESTIC ANIMALS
PRODUCTION, IMPORTATION, CONSUMPTION & DISPOSAL

A number of difficulties are encountered in this process of estimating concentrations from expected discharges.

1. The amount of chemical entering the environment may be a highly variable fraction of the amount actually manufactured or imported.

2. The nature of environmental fate depends on the pattern of discharge, i.e., whether the chemical is discharged to the air or soil environment, and the extent to which discharge is localized, i.e., whether discharge is diluted over a wide area and a large population or in a small area over a more highly exposed population.

3. With the present state of the art in environmental chemistry, it is difficult to calculate environmental rates of degradation by processes such as biodegradation, photolysis and oxidation. Calculated concentrations may thus be in serious error, especially for chemicals which have highly uncertain half lives.

4. A significant pathway for human exposure is consumption of vegetation, meat and dairy products. Our present ability to calculate concentrations in vegetation as a function of air and soil concentrations is severely limited; thus, estimations of this exposure pathway may be quite unreliable. Other complications are the widespread use of imported foodstuffs grown under entirely different environmental conditions and altered levels of contamination caused by food preparation techniques prior to human consumption.

5. It is difficult and possibly misleading to establish a typical Canadian diet since eating habits depend on lifestyle, geographic location and age. There are obvious and significant differences in dietary habits, especially in proportions of fish and domestically grown vegetation. However, it is not entirely clear how lifestyle differences can or should be factored into the assessment process.

Despite these difficulties, there is a compelling incentive to attempt the development of calculation procedures or models to process the available data and elucidate the nature and magnitude of the dominant exposure pathways. The process should be fairly simple and understandable so that users will not misapply estimating techniques. A training program could help familiarize them with the procedures used in a calculation. Because environmental fate and exposure calculations can be highly speculative and subject to error, there is obviously a need for validation and testing of whatever models are used, preferably using a variety of chemicals for which reliable data are available on discharge rates, environmental concentrations and extent of human exposure. However, the alternative of not using a model exposure procedure is even less acceptable since it would inevitably involve simple subjective judgement of the hazard associated with chemical purely from a knowledge of the input data. Within the next decade a number of models to measure environmental fate, human exposure and pharmacokinetics are expected to be able to perform these assessments with increasing reliability. The present review should be viewed as merely an attempt to guide activities in the meantime.

The primary focus of this report is on the assessment of organic chemicals rather than metals or metal-organic complexes. The number of metals is, of course, limited, and the more toxic metals have already been the subject of considerable environmental human toxicity assessment. Moreover, any proposal to market, for example, a cadmium compound would require a custom assessment takes into account the particular toxicological and environmental characteristics of cadmium compounds. General exposure models will be of less value in assessing compounds of this type. Models will also be of limited value for assessment of certain other classes of chemicals, notably polymers, surfactants, chelating agents, dyes and other molecules of very high molecular weight. They may also require individual assessment because certain physical or chemical properties such as vapour pressure, boiling point, solubility in water or octanol/water partition coefficient may not be in the range of normally measurable values.

1.2 Approach in this Report

Chapter 2 describes the literature search and agency contact procedure that sought out information on available models. From the pertinent references obtained (cited in the reference section) were selected some 20 models or modelling approaches deemed worthy of discussion. These are discussed individually in Chapter 2. Chapter 3 is a critical evaluation of the models, including a discussion of their nature, accuracy, acceptance, and availability. In Chapter 4 specific conclusions are reached and recommendations made for a modelling approach to be used by Health and Welfare Canada for assessing human exposure to new chemicals submitted under the Act.

2. Inventory of Model and Approaches

2.1 The Search Process

In recent years, a small community of model builders and model users have exchanged programs and reports so that each individual can exploit the refinements developed by other researchers. Information for this report was sought mainly through personal contact with these individuals or groups and scrutiny of appropriate literature. Notable meeting grounds have included two conferences arranged in Los Angeles by the National Center for Intermedia Transport Research at the University of California, Los Angeles and meetings of the American Chemical Society and the Society for Environmental Toxicology and Chemistry.

Contact was also made with groups such as the Environmental Protection Agency (EPA), Department of Energy and Army in the United States, the Michigan Department of Natural Resources, the Province of Ontario, and Lawrence Livermore Laboratories to obtain information on current and planned activities. It was encouraging that information was generally made freely available.

Considerable information was also gained from a Workshop, "Human Exposure to Chemicals," sponsored by the University of Toronto and the Ontario Ministry of Environment and held in Toronto in December 1988.

An invaluable source of information is the Compendium of Exposure Assessment Methods, recently compiled by the OECD Chemicals Group and Management Committee Hazard Assessment Panel. Table 2.1 is a reproduction of the Table of Contents of that report. Note that the report is designated Restricted.

The compilation of models and modelling approaches in Section 2.2 represents a fairly complete inventory of existing models. It must be emphasized that new models are expected to emerge in this dynamic area the next few years. Later in this report, recommendations are made for specific Health and Welfare activities to ensure that the Department remains up to date in this fast-developing field.

For convenience, the models are designated by letters A, B, C, etc., and presented individually with essential information and minimal contents. General comments and evaluation follow in Chapter 3.

Table 2.1
Draft compendium of environmental exposure assessment methods for chemicals.

General Table of Contents

		Page
PART 1	INTRODUCTION	5
	SUMMARY TABLE OF THE METHODS	13
PART 2	SOURCE ASSESSMENT METHODS	27
101	Product Category Approach	29
102	Assessment of the Environmental Releases of New Chemicals	32
103	Toxic Chemical Release Inventory	34
104	RLTEC Release from the Technosphere	37
105	Source Assessment Using Simple Dilution Models	42
106	Industrial Sources of Water Releases	47
107	Waste Water and Waste from Metal Plating	51
108	Environmental Information and Planning Model (RIM)	53
109	SIMPLETREAT	60
110	Environmental Risk Analysis	62
111	Model for Estimating Two-Phase Discharges of Liquified Gases Through Pipes – TPDIS	65
112	Model for Estimating Two-Phase Tubulent Jets – FLJET	69
PART 3	FATE AND PATHWAYS ASSESSMENT METHODS	75
	WATER METHODS	77
201	River Dilution Model	79
202	Dynamic Toxicity Model (DYNTOX)	85
203	Probabilistic Dilution Model – Version 3 (PDM-3)	88

Table 2.1 (cont'd)

204	Reach Scan	96
205	SARAH A Surface Water Assessment Model for Back Calculating Reductions in Abiotic Hazardous Wastes	104
206	QWASI Model River, Lake Modified	107
207	EXWAT	111
208	Model of Exposure Assessment in Water (MEXWA)	120
209	Geochemical Mass Balances	125
210	MUMM-MU-SLICK	129
211	MUMM-OPIA	132
212	Exposure Analysis Modelling System (EXAMS – Version 2.92)	135
213	Water Analysis Simulation Programme (WASP4)	146
214	Water Quality Model WAQUA	154
215	Density Currents Model – DISTRO	158
216	Xenobiotics Transport and Effect Model based on Detailed Simulation of Hydrodynamics – XTEM	161
217	Three-Dimensional Transport and Influence Model based on Detailed Simulation of Hydrodynamics (Simons-Koponen)	168
	SOIL (GROUNDWATER) METHODS	175
301	Pesticide Estimation Model – PSM	177
302	EXSOL	186
303	Pesticide Root Zone Model (PRZM)	195
304	Seasonal Soil Compartment Model – 4-layer Version (SESOIL-4)	198
305	ONZAT	206
306	SOLUTE	215
307	Analytical, Transient One-, Two- and Three Dimensional Model AT1230	218
308	FLOSA: Flow System Analysis	223
	AIR METHODS	225
401	Pesticide Emission and Dispersion Model	227
402	Airborne Pesticide Particles Dispersion Model	229
403	TA-Luft-Ausbreitungsmodell	242
404	EXAIR	247
405	User's Network for Applied Modelling of Air Pollution (UNAMAP)	253
406	MUMM-ATMOS	256
407	EXATM	259
	MULTIMEDIA (MACKAY'S FUGACITY APPROACH) METHODS	265
501	Multimedia Fugacity Models	267
502	Assessment of Risk to Aquatic Biota	275
503	Environmental Exposure Potentials (EEP)	279
504	Fugacity Model (Levels I and II) – Modified	290
505	ENPART – The Environmental Partitioning Model	294
506	SIMPLESAL	307
507	Multi-phase Non-Steady State Equilibrium Model – Version 1.3 (MNSEM 1.3)	318
	MULTIMEDIA (OTHER APPROACHES) METHODS	329
601	SIMPLEBOX	331
602	EXINT	337
603	MINTEQAI Equilibrium Metal Specification Model	343
604	TOXSCREEN	346
605	Simulation for Water Resources in Rural Basins (SWRRB)	366
606	Hydrological Simulation Programme FORTRAN (HSPF)	368
607	Water Quality Assessment: A Screening Procedure for Toxic and Conventional Pollutants in Surface and Groundwaters	373
608	Contaminant Transport (EnviroTIPS Manual 1985)	376
ANNEX I	NOTES FOR PREPARING CONTRIBUTIONS (SOURCE ASSESSMENT METHODS)	383
ANNEX II	NOTES FOR PREPARING CONTRIBUTIONS (FATE AND PATHWAYS ASSESSMENT METHODS)	397
ANNEX III	LIST OF NATIONAL CONTACT POINTS	413

2.2 Inventory of Models

Model A

Name:
GEOTOX.

Type of Model:
Multimedia Exposure Model.

Reference:
McKone, T.E., Layton, D.W. "Screening the potential risks of toxic substances using a multimedia compartment model: Estimation of human exposure", Regulatory Toxicol. Pharmacol. 6:359-380, 1986.

Contact:
Dr. Tom McKone, Risk Assessment and Environmental Policy, Lawrence Livermore Laboratory, P.O. Box 5507, L-453, Livermore, CA 94550, USA, Telephone: (415) 422-7535.

Description:
GEOTOX is a comprehensive, multimedia, compartmental model developed under contract from the US Department of Energy and the US Army, which calculates chemical partitioning, degrading reactions and interphase transport of both diffusive and non-diffusive types. The concentrations estimated for various environmental compartments are combined with appropriate human inhalation and ingestion rates and absorption factors to calculate exposure.

GEOTOX incorporates an evaluative environment, representative of the Southeastern United States, consisting of the following compartments: air (gas), air (particles), biomass, upper soil, lower soil, groundwater, surface water and sediments. These media are assumed to be made up of sub-phases of gas, liquid and solid. Figure A.1 illustrates compartments and pathways included in the model. Environmental dimensions and characteristics can be adjusted to represent other regions.

Chemical partitioning between compartments, interphase transport, reaction and advective losses are described by first-order rate constants. The model consists of a set of simultaneous differential equations in matrix form, which can be solved for constant or time-varying chemical sources.

The atmosphere, which is in contact with the soil and water, is considered to consist of a vapour and particulate (i.e., aerosol) phase. Input to this compartment may be from a point source or by diffusive transfer (volatilization) from soil and water. Chemical leaves the compartment by advection or reaction, or in association with wet and dry particle deposition.

The soil compartment is treated as three layers: uppersoil layer, lower soil layer and groundwater zone. The upper and lower soil layers are described by parameters of depth, bulk density, porosity, water content and fraction organic carbon. The groundwater compartment consists of solids and fluids, that is, all the pore spaces are occupied by water. Chemical is removed from the upper soil layer by volatilization, runoff, plant uptake and downward leaching. Removal from the lower soil layer is mainly by downward leaching. Transport in the groundwater is horizontal. Processes of adsorption, ion exchange, precipitation, colloidal infiltration and irreversible mineralization in the groundwater are incorporated by means of appropriate sorption partitioning constants and expressions.

The water phase is considered to consist of water, biota and suspended solids in equilibrium. Solids enter the water by atmospheric deposition and surface erosion and leave by advection and sedimentation. Liquids enter by runoff, rainfall and groundwater discharge and leave by advection and sedimentation. The bottom sediment compartment consists of solids and pore water. Chemical entry and removal are by diffusion, deposition and resuspension.

Concentration in land biomass is calculated as the product of the soil concentration and plant-soil partition coefficient, i.e., an equilibrium type of expression is assumed incorporating vegetation production or growth rate. Animal biomass is not considered in the mass balance but it is treated as an exposure vector.

Both abiotic and biotic transformation processes are included as first-order rate constants. If no rate constant is available, the parameter is set to zero to reflect a conservative estimate.

Environmental dimensions and characteristics can be adjusted to represent other regions. Human exposure pathways considered are inhalation of air; ingestion of fruit, vegetables and grain; ingestion of meat, milk and dairy products; ingestion of fish; ingestion of soil; and dermal absorption.

The following assumptions are included in the assessment of human exposure:

i) Inhalation exposure considers chemical in both gaseous and particle phase. For the vapour phase, exposure is assumed to take place over the whole year. Exposure through the particulate phase is assumed to occur only when ground is not covered by standing rainwater or snow.

ii) Drinking water is assumed to come equally from surface and groundwater.

iii) Vegetation is assumed to be mainly from crops (i.e., fruits, vegetables and grains) grown in neighbouring regions.

iv) Contamination of cattle through air inhalation and water, vegetation and soil ingestion is calculated by means of a partition coefficient to animal fat. Figure A.2 is an illustration of the cattle/meat/dairy/human pathways.

v) Fish consumption is treated using a conventional fish bioconcentration factor.

vi) A term for soil ingestion by humans is included. It varies according to age.

vii) Dermal sorption is considered to be from contact with soil only. This process is not quantified for swimming or bathing.

viii) Exposure is modified according to age group.

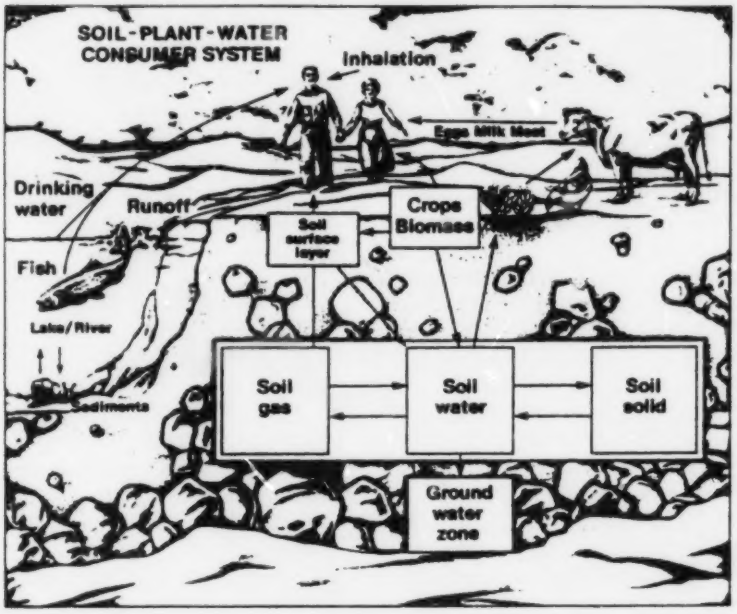


Figure A.1
Conceptual diagram of the major compartments, phases and pathways addressed in the screening methodology.

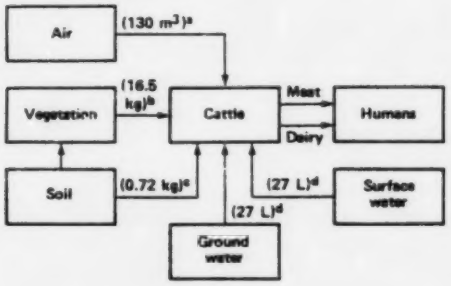


Figure A.2
Schematic of the cattle/meat/dairy product pathway model.
(All values are daily intake. [a]Anspaugh et al. (1971). [b]Dry mass intake of vegetation (Rosenblatt et al., 1983). [c]Ingestion of soil by cattle (Small, 1984). This value is probably somewhat high. Smith (1977) reports that a reasonable estimate of soil ingestion is in the range 0.25 to 0.5 kg/day. [d]Total water consumption is 55 liters/day (USNRC, 1977), we assume that intake is equally divided between surface and soil water.)

The average dose rate is calculated as the average of the time integral of daily intake over all pathways. A term is included to reflect the fraction of the year in which exposure occurs. An absorption factor is also included, although this factor is not well quantified.

Relative risks of chemicals are estimated by comparing estimated dose rates to Virtually Safe Dose Rates (VSDR). Table A.1 illustrates environmental distribution and resulting exposure for unit releases of chemicals. Relative risks are assessed. This method is valuable primarily as a screening tool. However, the model could be adapted to other specific regions.

Data Requirements:

Physical chemical properties: solubility, vapour pressure, K_{OW}. Degradation rate constants. Emission data. Environmental characteristics, including fraction of land surface covered by water and average water depth.

Output:

Output is in the form of environmental concentrations, intake by various exposure pathways and total intake. Relative health risk for a number of chemicals can be calculated.

Applications:

GEOTOX has been applied to assess relative health risks of three chemicals: 2,4,6-trinitrotoluene, hexahydro-1,3,5-trinitro-1,3,5-triazine, and benzene. A "unit exposure analysis" is used, which assumes a continuous unit input to the upper soil layer. Resulting exposures are compared with Virtually Safe Dose Rates (VSDR) and ranked according to proximity to this dose rate, as illustrated in Tables A.1 and A.2.

Computer:

Available on 5 diskettes for IBM hard disk.

Availability:

Disks are available from Lawrence Livermore at no cost. A licence agreement regarding copying of disk must be signed.

Comments:

This is one of the most advanced models in existence. It contains virtually all the key components of a complete exposure analysis. The authors acknowledge the weakness of the plant uptake expressions. The group is still active in this area and it is expected that new versions will be produced in the near future.

Table A.1
Daily doses predicted for the seven exposure pathways after the release of 1 mol/km^2-year of each contaminant into the upper soil compartment.

	Absorbed dose (mg/kg.day)		
Pathway	Benzene	RDX	TNT
Inhalation	3×10^{-7}	2×10^{-11}	2×10^{-8}
Water consumption	5×10^{-10}	1×10^{-5}	1×10^{-5}
Fruit and vegetable ingestion	4×10^{-10}	4×10^{-5}	1×10^{-5}
Meat and dairy ingestion	2×10^{-10}	6×10^{-8}	7×10^{-8}
Fish ingestion	6×10^{-10}	7×10^{-8}	6×10^{-8}
Scil ingestion	3×10^{-14}	5×10^{-11}	4×10^{-10}
Dermal absorption	2×10^{-14}	3×10^{-12}	2×10^{-10}
Totals	3×10^{-7}	5×10^{-5}	2×10^{-5}

Table A.2
Comparison of estimated contaminant dose rates from all exposure pathways and Virtually Safe Dose Rates (VSDR).

Contaminant	Dose rate (mg/kg.day) A	VSDR (mg/kg.day) B	Screening ratio A/B	Rank
Benzene	3×10^{-7}	4×10^{-5} [a]	7.5×10^{-3}	2
TNT	2×10^{-5}	1×10^{-3} [b]	2×10^{-2}	1
RDX	5×10^{-5}	1×10^{-2} [c]	5×10^{-3}	3

[a]Based on a lifetime leukemia risk of 10^{-6} (derived from Layton *et al.*, 1981).
[b]Calculated from a drinking-water standard of 0.05 mg/litter (National Research Council, 1982).
[c]Calculated from a chronic no-observed-effect level of 1 mg/kg.day in laboratory animals (National Research Council, 1982) and a safety factor of 100.

Model B

Name:

Remedial Action Priority System (RAPS).

Type of Model:

Hazardous Waste Site Multimedia Exposure Model.

Reference:

Whelan, G., Strange, D.L., Droppo, J.G., Jr., Steelman, B.L. Buck, J.W. "The remedial action priority system (RAPS): mathematical formulations", prepared for the U.S. Department of Energy, Office of Environment, Safety and Health, 1987.

Contact:

Dr. James G. Droppo, Jr., Pacific Northwest Laboratories, P.O. Box 999, Richland, WA 99352, USA, Telephone: (509) 376-7652.

Description:

The RAPS system was prepared for the U.S. Department of Energy for hazard ranking of chemical and radioactive waste disposal sites. It is used primarily as a tool for setting priorities for site investigation and possible remediation. It is intended to be used in a comparative rather than predictive mode. The methodology considers four major pathways of contaminant migration: groundwater, surface water, overland and atmospheric. Resulting estimated concentrations in the air, soil, sediments and water are used to assess exposure to neighbouring populations.

The detailed exposure assessment considers exposure through: inhalation of airborne pollutants; ingestion of contaminated drinking water, fish and shellfish, vegetation and animal products; external doses from radiation; and external dermal contact with chemicals. Total exposure through all routes is estimated and combined with toxicity data to calculate a hazard potential index (HPI).

The "pseudocomposite" multimedia methodology calculates only independent modules, which do not interact spatially or temporally; that is, transfer of pollutant is in one direction only. This modular framework permits updating, or inclusion of additional components with advancing technology.

RAPS employs user-supplied data on site and pollutant characteristics to simulate migration and fate from source to receptor by various pathways. The user must identify appropriate routes of chemical from waste site to neighbouring populations through various media. Exposure is calculated in terms of a lifetime dose. Once exposure has been assessed, an HPI is calculated for the site. The four environmental pathways and resulting exposure routes are illustrated in Figure B.1, with shaded boxes representing an example of transport and exposure routes.

Contaminants leaching from soil, landfill or ponds migrate through a partially saturated or saturated groundwater zone. Movement in the partially saturated zone is assumed to be vertical, while movement in the saturated zone is in the direction of groundwater flow. The groundwater module calculates concentrations at neighbouring wells and river edges, as well as flux to the surface water. The potential coupling of the groundwater and other modules is illustrated in Figure B.2.

Surface water bodies typically might include non-tidal rivers, estuaries, lakes, open coasts and impoundments. However, at this stage of development, RAPS includes only non-tidal rivers. Additional water bodies may be added as independent modules when necessary. Since the residence time of short-term releases of chemical may be shorter than the time for distribution in surface waters, only continuous, steady-state releases are considered. The surface water module considers transport by advection and dispersion. Interaction with other modules is illustrated in Figure B.2.

Overland flow, resulting mainly from precipitation, is the fraction seen as flowing water on the ground surface. Estimation of contaminant flow is based on information on soil type and cover, land use and treatment, hydrologic conditions, location, and soil moisture content. Direct runoff from storms can be estimated. Soil erosion is considered for different geographical and vegetative conditions. Exposure by this route is described in Figure B.2.

RAPS considers release mechanisms and characteristics, dilution and transport, washout and precipitation, and dry deposition in the atmospheric pathway. Degradation is not considered because contaminant transport is assumed to be rapid. This provides a conservative estimate.

Human exposure routes are illustrated in Figure B.3.

The inhalation route includes inhalation of ambient air as well as of contaminated vapour while showering. Populations within 80 km of the site are potentially exposed by the atmospheric pathway. Exposure from contaminated air is calculated from the breathing rate and average air concentration. The shower pathway is considered for groundwater only as volatile compounds presumably have a short half-life in surface or overland water.

The calculation of exposure from drinking water considers contamination by groundwater, overland and surface water pathways. The dose is calculated from the water concentration, water ingestion rate, a water treatment factor and a decay factor, where applicable, for radioactive decay or degradation.

Ingestion of aquatic food considers both fish from free-flowing waters and shellfish living in sediments. This exposure pathway is considered for surface and overland transport pathways. Dose is calculated from water concentration and bioconcentration factor.

Figure B.1
Simplified diagram outlining the interactions between the transport pathways and exposure assessment components of the RAPS methodology (shaded boxes indicate a potential contaminant transport and exposure route using the RAPS methodology (after Whelan *et al.* 1986)).

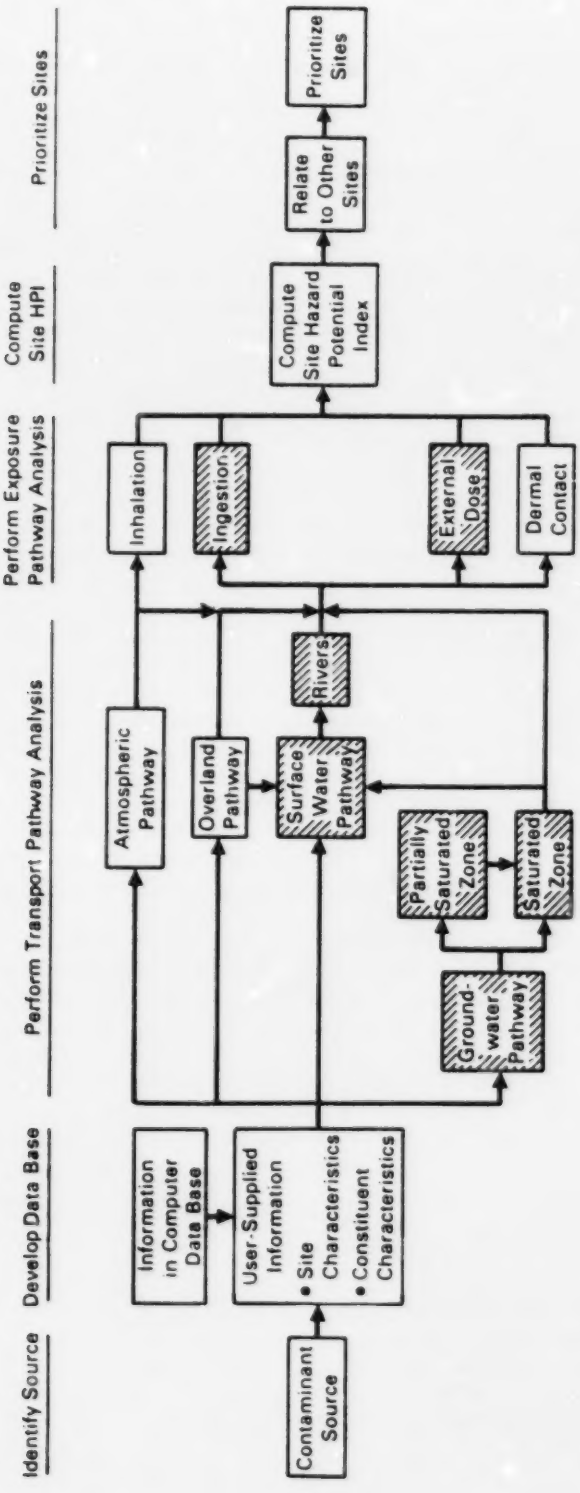


Figure B.2
Exposure pathways considered by RAPS (after Bolten *et al.* 1983; Whelan *et al.* 1987).

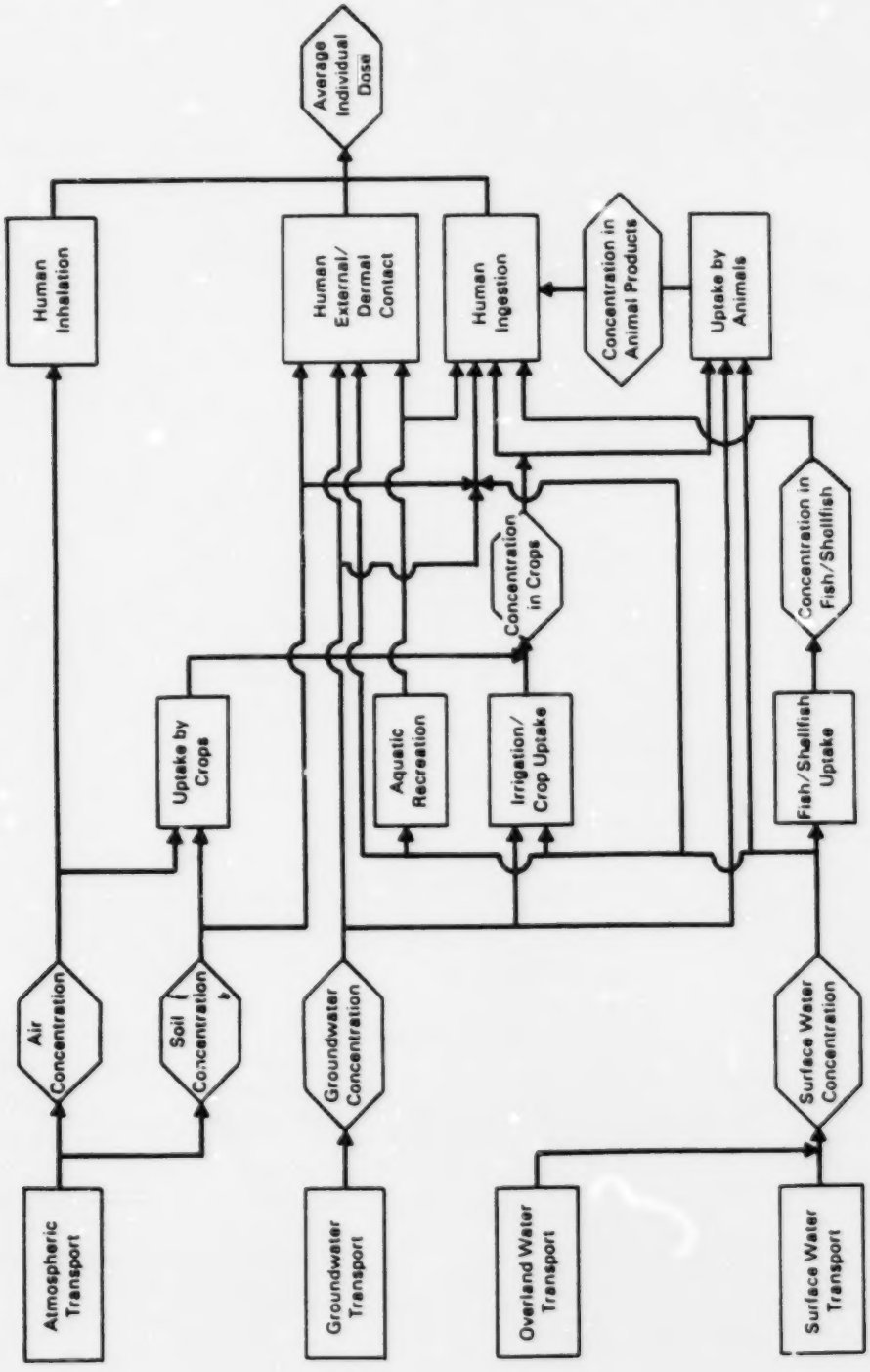
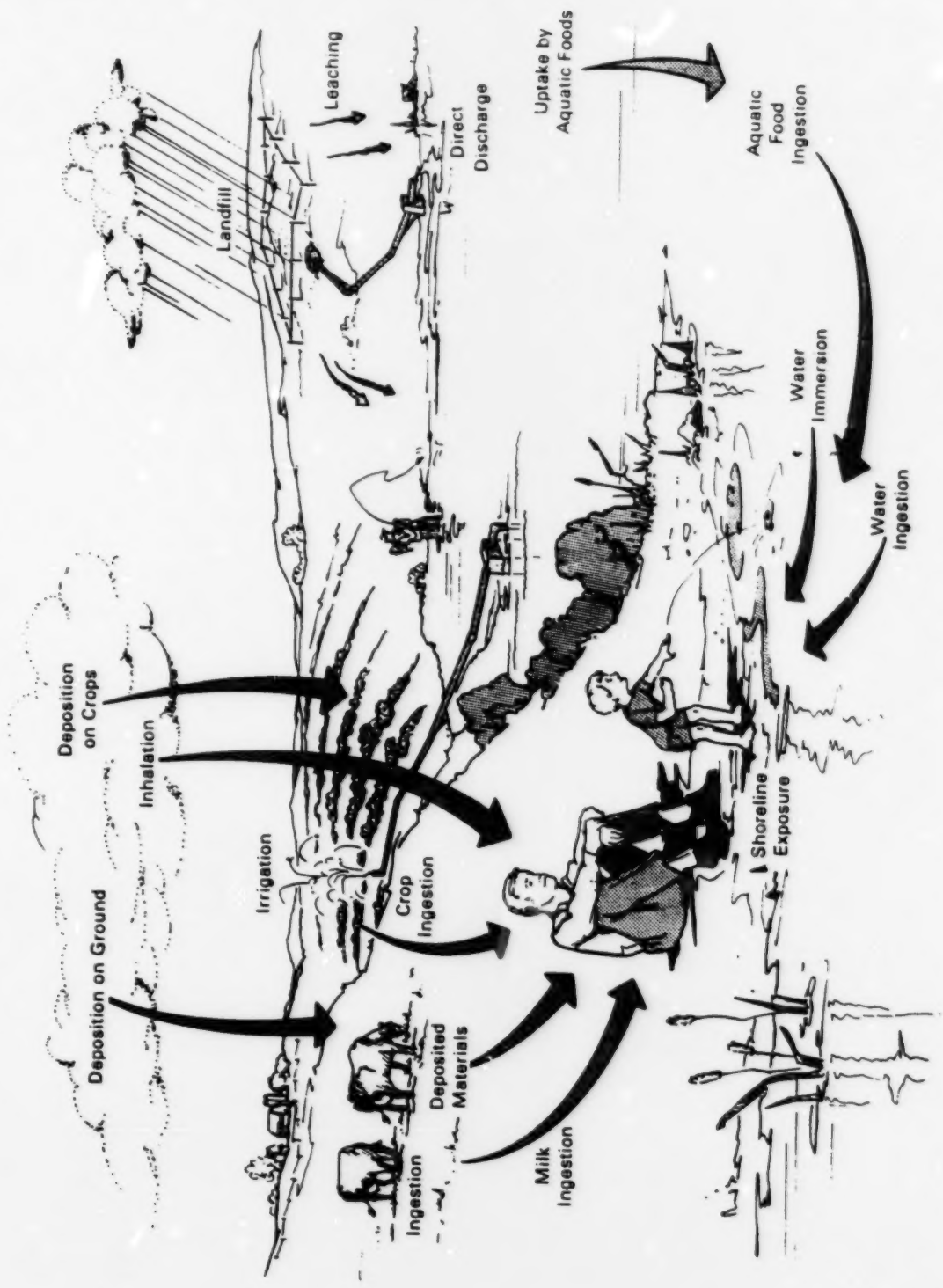


Figure B.3
Exposure pathways to humans



Contamination of crops by irrigation is considered as well as by atmospheric deposition and root uptake. Two categories of vegetation are considered, leafy and other. "Leafy" includes lettuce and other vegetation with edible portions above ground. "Other" represents those whose edible portions are not contaminated in a major way by direct deposition. Plant concentration due to direct deposition is calculated from plant type, deposition rate, possible decay and degradation rate constants, residence time of particle on plant, and a translocation factor. Contamination due to irrigation is calculated from an irrigation rate and water concentration. Soil-to-plant transfer is not well quantified and is calculated by means of a regression correlation with octanol/water partition coefficient, KOW. Total plant concentration is calculated as the sum of these processes. Concentrations resulting from irrigation and atmospheric contamination are based on a one-year farming cycle. For contribution from uptake from soil, a correction is made for year-to-year accumulation in soil. Exposure is estimated from concentration and average consumption rates for the two types of vegetation.

Chemical intake by domestic animals is assumed to result from ingestion of contaminated feed, water used to irrigate feed, and drinking water. Animal products considered are beef and cow's milk. Concentration in feed is vegetation concentration modified to represent a shorter growing period to reflect grazing habits. Transfer coefficients to meat and milk are calculated from available correlations with K_{OW}. Like soil-to-vegetation transfer correlations, they give only approximate estimates.

Inadvertent ingestion of soil and water is also estimated. Dermal absorption through skin is not considered since this is assumed to be minor in comparison to the conservative estimate of inadvertent ingestion of soil and water.

External exposure to radiation from chemicals from aquatic recreational activities is estimated as is exposure to contaminated soil or shoreline sediments from overland activities such as hiking or shoreline fishing. Estimation of exposure includes consideration of soil or water concentration, time spent in the activity, water immersion dose factors, and concentration of contaminated sediment deposited on shore.

Total exposure through all routes is estimated and combined with toxicity data. An individual risk factor is compiled for radionuclides, and for carcinogenic and non-carcinogenic chemicals. Those risk factors are combined with population exposed and a time factor to determine the HPI. Sites are then ranked in increasing order of HPI. Use of site-specific information reduces subjectivity.

Data Requirements:

Data requirements include detailed site-specific information on hydrological and soil characteristics, climate and meteorological conditions, as well as contaminant characteristics. Input must include identification of possible exposure routes.

Output:

Output is in the form of environmental concentrations and exposure potential through various pathways.

Lifetime exposure to neighbouring populations from all pathways considered is calculated and an HPI is compiled for the site.

Applications:

Applications have been published only for hypothetical cases involving arsenic and strontium 90.

Computer:

Extensive mainframe-based.

Availability:

Not known, but key expressions have been published.

Comments:

This model is not directly suitable for assessment of human exposure to chemicals in general commercial use. It is primarily aimed at ranking waste sites for remediation under US Superfund legislation. Its strength and usefulness is that a great deal of effort has been devoted to establishing reasonable expressions for transport and exposure. These could be profitably exploited in the development of new models, i.e., modules could be adopted as required.

An enhanced version of RAPS has been developed recently by Battelle for the US Department of Energy. A summary of this multimedia environmental pollutant assessment system, or MEPAS, is appended to this section.

MEPAS: New Approach to Managing Environmental Problems

As our understanding of the effects of industrialization on public health and the environment has increased, the number of recognized environmental problems has grown dramatically. Scientifically based assessment methodologies are needed to help develop environmental management strategies to address this growing list of problems. For example, assessment methodologies for potential contaminant exposure levels and the associated health and environmental risks can be used to assign relative rankings to these problems.

In the past, contaminant assessments generally focused on only one environmental pathway, such as groundwater, surface water, or the atmosphere. However, in the real world, contaminants released into one medium eventually migrate through and interact with several media. For example, atmospheric contaminants from a stack are deposited onto the surrounding land surface, then transported overland through precipitation to the surface water, and finally to groundwater through soil leaching. Thus, to more accurately portray the complexities of the interactions of contaminants and the environment, scientifically based assessment methodologies must consider integrated multimedia transport and contaminant fate.

Once potential environmental problems have been identified, they must be ranked to address first those problems with greatest overall potential impacts. Contaminant arrival time and exposure duration are important considerations in assessing potential effects on public health and the environment. To adequately address these concerns, a scientifically based, defensible ranking methodology should be used early in the investigation. This methodology would focus on available human and financial resources for further investigation and possible remediation of high-risk problems.

Risk-Based Prioritization Using MEPAS

The U.S. Department of Energy (DOE) Office of Environment, Safety, and Health is conducting an environmental survey of the entire DOE complex to identify and assign priorities to potential environmental problems. A strong, technically based method was needed to assign priorities to DOE's environmental problems to ensure efficient long-range planning of corrective actions. The methodology also had to be versatile enough to encompass a full range of environmental media and pollutant scenarios. DOE turned to the researchers at the Pacific Northwest Laboratory (PNL), who developed the Multimedia Environmental Pollutant Assessment System (MEPAS).

MEPAS is an enhancement of the Remedial Action Priority System (RAPS), which was also developed by the laboratory for DOE. MEPAS ranks environmental problems according to risk to human health. It is an objective, physics-based, fully integrated, multimedia environmental assessment system. MEPAS is a computer-based system that uses empirically, analytically and semi-analytically based mathematical equations. MEPAS methodology uses generally accepted, independently peer-reviewed computer models. The pathway analysis simulates the potential release of contaminants into the environment, transports the contaminants through and between multiple environmental media, exposes surrounding populations to them, and computes health effects (i.e., risk) associated with the exposure.

Unlike more complex assessment models, MEPAS uses readily available data at early stages of problem investigation. MEPAS can be operated using contaminant source-term data from the type of site inspections conducted under the Comprehensive Environmental Response, Compensation, and Liability Act. Data concerning the environmental setting for the problem can be supplied either from site-specific records or from federal, state and local agency publications and records.

MEPAS addresses many of the typical constraints associated with screening methodologies and thereby serves as a bridge between the environmental problem screening process and the more resource-intensive site characterizations and quantitative assessment. Using MEPAS, investigators can

- address both chemical and radioactive waste
- use site-specific information for a more accurate assessment
- define the problem, input data, and operate MEPAS through a user-friendly shell
- consider the contaminant characteristics associated with transport through the pathways, including such factors as retention and arrival time at sensitive receptors
- calculate the various routes of exposure, including inhalation, ingestion, dermal contact, and external doses, while factoring the duration and level of exposure to the size of the population risk.

Because environmental problems are not necessarily limited to long-term inactive release, MEPAS also is designed to address shorter term, transient (i.e., batched or infrequent) releases, such as those from atmospheric stack emissions or fallout discharge to surface water bodies. These additional features allow the system to provide an assessment of environmental problems that cross regulatory lines, thus providing a common, objective basis for assigning priorities to a vast array of environmental situations.

User-Friendly Shell

For most computer models, inputting and checking the required data for a given transport and exposure scenario is tedious and time-consuming. Because of this, researchers at the Pacific Northwest Laboratory designed an interface for the MEPAS user that allows easy data entry, quality control checks on the entered data, and easy batch mode running of the MEPAS models.

To implement MEPAS for a site, the investigator designates appropriate transport pathways by identifying the path of the constituents from the waste site through the various media. The investigator is then prompted to supply site and constituent information. The exposure routes to the population are integrated into the analysis, and the subsequent risk to the population is computed for the site.

The user-friendly shell provides easy access and manipulation of the site data and files for assessing hazardous waste sites. MEPAS operates on a IBM-PC for 100% compatible) with 640K RAM and a 20-Mb hard disk. It uses a 132-column printer. A math coprocessor is not required, but it will greatly improve model performance. The data capture and storage programs are written in compiled dBase III Plus. The MEPAS model is in FORTRAN, and intermediate programs are in C. Installation requires approximately 1 Mb of disk space. This is a file-based application; all data are stored and exchanged between major components by file input/output.

The user-friendly shell provides menu options to assess the following components:

- Create/Update/Examine – The investigator defines a potential environmental problem and enters the data required to operate the model. This definition is used to develop problem-specific worksheets of required source term, transport pathway, and exposure pathway data. Previously entered problems and data can be used to create new runs.

- Run/Print Reports/Templates – The investigator operates the MEPAS model for the environmental problem defined in the previous step. Documentation of inputs and outputs may be printed from this component.
- Constituent Library – A fast-search module allows the investigator to quickly view the physical and chemical properties of radionuclides and chemicals used in the MEPAS model.

Applications of the Model

The MEPAS model is currently being used by DOE for the environmental survey of all DOE facilities across the nation. This includes 16 defense production facilities as well as 20 other major DOE operating facilities. Approximately 500 ranking units from these facilities are being assessed using MEPAS. A ranking unit is a related group of environmental problems at a site.

The MEPAS model has also been used for 20 U.S. Environmental Protection Agency (EPA) Superfund sites as part of an effort by the EPA to address the intent of the Superfund Amendments Reauthorization Act (SARA). A comparison of MEPAS with the revised hazard ranking system (HRS) showed MEPAS to be a viable ranking technique.

In addition to ranking sites, MEPAS has been applied to problems at one site, where a relative ranking of the constituent pathways at a site was obtained. This relative ranking was used to assess the appropriate actions at this site.

About Pacific Northwest Laboratory

Operated by Battelle Memorial Institute, the Pacific Northwest Laboratory is one of the U.S. Department of Energy's five multiprogram national laboratories. The Laboratory, which also conducts research programs for other government agencies, develops and deploys technology to support national missions for energy, defense, and economic competitiveness.

Additional information about the MEPAS methodology is available from the Pacific Northwest Laboratory. For more information contact:

Dr. James C. Droppo, Jr.
(509) 376-7652
John W. Buck
(509) 376-3442

Pacific Northwest Laboratory
P.O. Box 999
Richland, Washington 99352

Model C

Name:

Multi-phase Non-steady State Equilibrium Model (MNSEM).

Type of Model:

Multimedia-Compartmental Model.

Reference:

i) Yoshida, K., Shigeoka, T., Yamauchi, F. "Estimation of environmental fate of industrial chemicals", Toxicol. Environ. Chem. 17:69-85, 1988.

ii) Method 507, Draft Compendium of Environmental Exposure Assessment Methods for Chemicals, OECD Chemicals Group and Management Committee, Hazard Assessment Panel (in press 1988).

Contact:

Dr. Kikuo Yoshida, Environmental Science Division, Mitsubishi-Kasei Institute of Toxicological and Environmental Sciences, 1000 Kamoshida-cho, Midori-Ku, Yokohama 227, Japan, Telephone: 045-963-3543.

Description:

MNSEM is a kinetic model designed to predict the environmental fate of organic chemicals under steady-state conditions of continuous loading to the environment. It calculates the chemical distribution, persistence and concentrations in an evaluative or hypothetical environment consisting of "reasonable" volume ratios of environmental media. It also estimates recovery time after emissions are terminated.

The model environment, representative of Japan, consists of four major compartments: air, water, soil and sediment, with subcompartments of air and raindrops in air; biota and suspended solids in water; air, water and solids in soil; and pore-water solids in sediment. As in the fugacity models, each phase is well mixed and equilibrium is assumed to exist within but not between compartments. The mass balance set of differential equations includes expressions for diffusive and non-diffusive interphase transfer and degradation processes. Intraphase partitioning is described in terms of equilibrium constants including organic carbon partition coefficient, KOC, bioconcentration factors (BCF) and Henry's Law Constant, H.

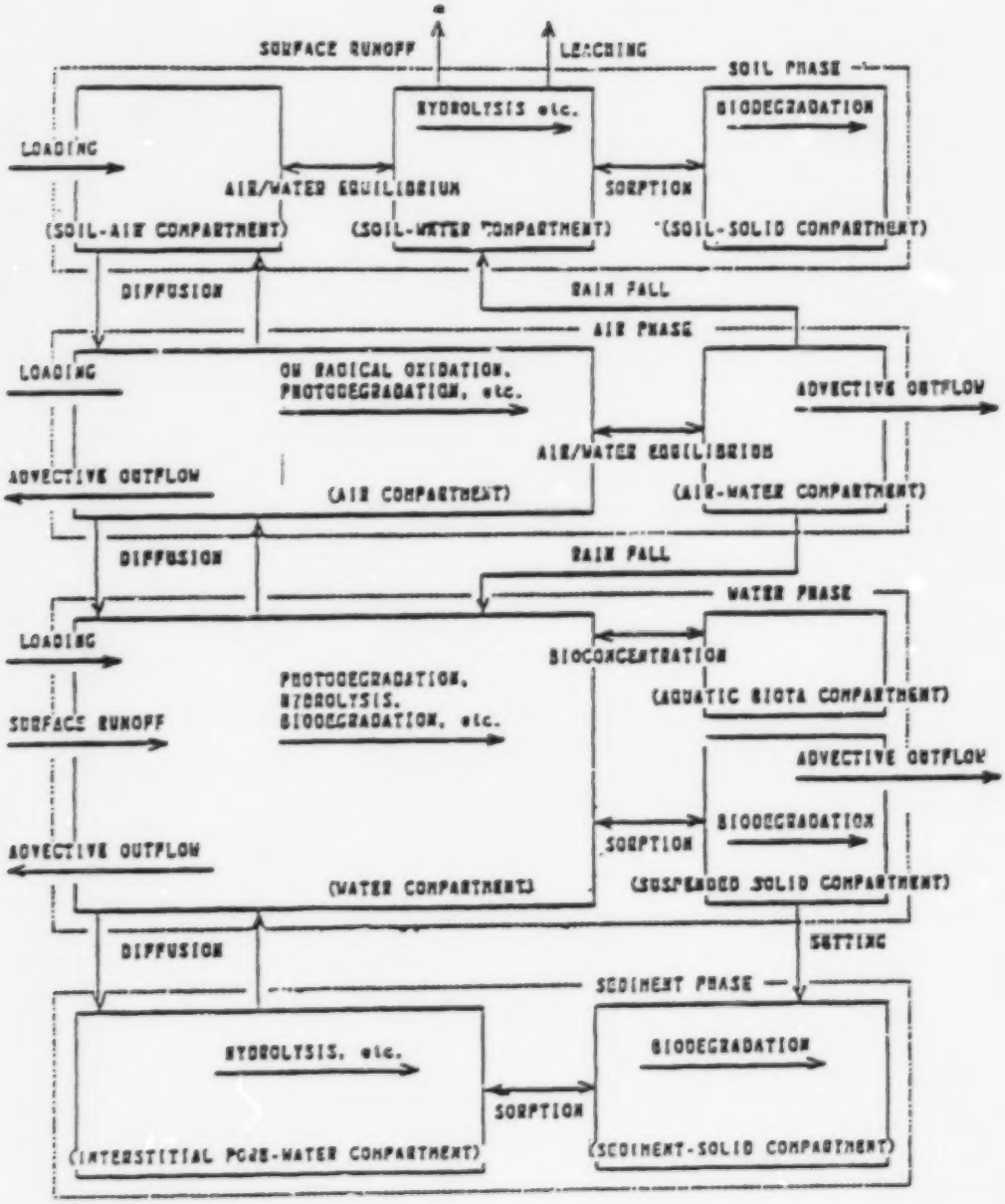
Interphase diffusive transfer between air and soil, air and water, and sediment and water is quantified by means of mass transfer coefficients. Non-diffusive transfer processes of rainfall, surface runoff, suspended sediment deposition and leaching from soil are characterized by rate constants. Degradation processes include hydroxy radical oxidation, photolysis, hydrolysis and biodegradation.

These processes are illustrated in Figure C.1.

The model estimates steady-state concentrations in each phase and clearance time in the environment.

MNSEM is not a site-specific model and temperature dependence of physical chemical properties is not considered.

Figure C.1
Schematic diagram of environmental fate



Data Requirements:

Input data requirements include solubility, vapour pressure, organic carbon sorption coefficient (K_{OC}) and bioconcentration factor (BCF). There is no default calculation for K_{OC} and BCF. Data on transformation rate constants and chemical loading rates are also required. Loading rates are estimated from annual production in Japan, use patterns and physicochemical properties. This algorithm is not included in the model.

Applications:

The model has been applied to the fate of chloroform, aniline, chlorobenzene, nitrobenzene and naphthalene in Japan. Estimated concentrations are generally within an order of magnitude of available data. A summary of the estimated environmental fate of napthalene is given in Table C.1.

Computer:

Program is written in Microsoft MS-DOS BASIC and is available on a floppy disk.

Availability:

Contact Dr. Yoshida.

Comments:

This model is of particular interest because the motivation behind it is similar to that of CEPA in Canada. It treats an entire country. It is very encouraging that the model has been successfully applied in Japan. Estimated concentrations are within an order of magnitude of observed concentrations, which is probably as good as can be expected, given the spatial variability in concentrations influenced by proximity to urban or industrial areas.

Table C.1
Summary of environmental fate of naphthalene, evaluated by multi-phase non-steady state equilibrium model (version 1.3).

1. Mass Distribution Fraction

Air Phase	
• Air compartment	% : 99.83
• Air-water compartment	% : 0.17
Water Phase	
• Water compartment	% : 99.94
• Suspended solid compartment	% : 0.05
• Aquatic biota compartment	% : 0.01
Soil Phase	
• Air compartment	% : 0.01
• Water compartment	% : 0.92
• Soil solid compartment	% : 99.07
Sediment Phase	
• Water compartment	% : 1.37
• Sediment solid compartment	% : 98.63

2. Mean Residence Time

Air Phase

Mean residence time : 0.783 day

Process	Rate Constant (1/day)	Contribution to Removal (%)
• Advective out flow	: 2.40E-01	18.79
• Transformation	: 1.02E+00	79.73
• Diffusion to water	: 1.82E-02	1.42
• Diffusion to soil	: 5.88E-04	0.05
• Rain fall	: 1.00E-01	0.01

Water Phase

Mean Residence Time : 6.756 day

Process	Rate Constant (1/day)	Contribution to Removal (%)
• Advective out flow	: 9.60E-03	6.48
• Transformation	: 1.89E-02	12.77
• Diffusion to air	: 5.96E-02	40.24
• Diffusion to sediment	: 6.00E-02	40.48
• Setting to sediment	: 1.00E-01	0.04

Soil Phase

Mean Residence Time : 37.090 day

Table C.1 (cont'd)

Process	Rate Constant (1/day)	Contribution to Removal (%)
• Transformation	:	33.47
(Water compartment	: 9.10E-04)	
(Soil solid compartment	: 9.10E-03)	
• Diffusion to air	: 1.57E+02	61.09
• Runoff to water	: 8.00E-02	2.72
• Leaching	: 8.00E-02	2.72

Sediment Phase

Mean Residence Time : 2.674 day

Process	Rate Constant (1/day)	Contribution to Removal (%)
• Transformation	:	2.40
(Water compartment	: 9.10E-04)	
(Sediment compartment	: 9.10E-03)	
• Diffusion to water	: 2.66E-01	97.60

3. Loading Rate to Environment, g/day

Air	: 29.00
Water	: 45.00
Soil	: 0.00

4. Steady State Solution

Phase	Mass	Concentration
Air	: 4.66E+01	2.33E-08 mg/L
		4.44E-06 ppm
Water	: 5.12E+02	7.32E-05 mg/L
Soil	: 1.10E+00	3.68E-05 mg/L
Sediment	: 8.22E+01	3.91E-03 mg/L

5. Clearance Time in the Environment

Clearance time : 3.10E+01 days

Model D

Name:
Persistence.

Type of Model:
Aquatic Model.

Reference:

i) National Research Council of Canada (NRCC). A screen for the relative persistence of lipophilic organic chemicals in aquatic ecosystems. An analysis of the role of a simple computer model in screening. Report of the NRCC's Associate Committee on Scientific Criteria for Environmental Quality. NRCC 18570, 1981.

ii) Asher, S.C., Lloyd, K.M., Mackay, D., Paterson, S., Roberts, J.R. A critical examination of environmental modelling - modelling the fate of chlorobenzenes using the persistence and fugacity models. NRCC's Associate Committee on Scientific Criteria for Environmental Quality. NRCC 23990.

Contact:

The developing group at NRCC is now disbanded. The primary author, J.R. Roberts, is now in an unrelated civil service function. K. Lloyd can be contacted at the Canadian Wildlife Service.

Description:

The persistence model was developed for the National Research Council of Canada as a screening tool to produce a systematic method of comparing predicted fates of various organic chemicals, especially pesticides, which may enter the aquatic environment. The model considers four compartments illustrated in Figure D.1: water, catch-all (representing suspended solids, invertebrates or other components of water system excluding fish), sediment and fish.

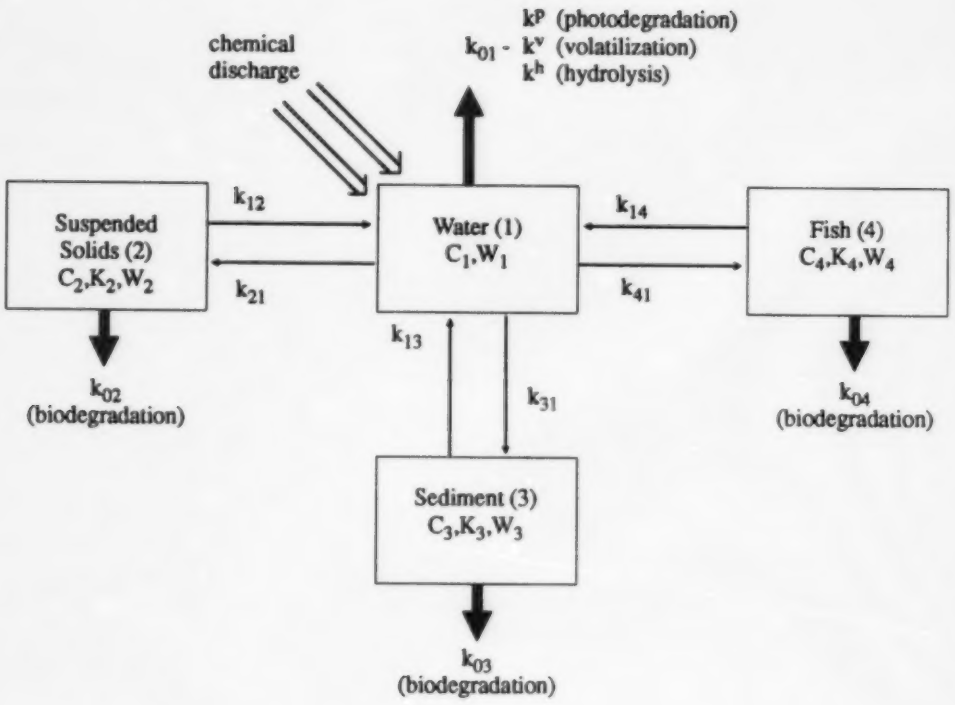
An air compartment is not specifically included but is treated as an infinite sink where chemical evaporated from water is permanently removed from the system. This limits the application of the system to small bodies of water where advection is dominant. Default environments for the model are a standard pond, simulating a small, eutrophic pond, and a standard lake simulating a deep, oligotrophic lake.

Chemical can be added to the water compartment only and can occur by finite release, continuous release, or pulses occurring over a period of time.

Transfer between water and the other three compartments is characterized by a rate constant. Degradation removal pathways included are photodegradation, volatilization, and hydrolysis in water; biodegradation in fish; and microbial degradation in suspended solids and sediments.

The dynamic solution, calculated from a set of differential equations, estimates concentration as a function of time. An overall "retentive capacity" or persistence is calculated. The output can be in graphic or tabular form.

Figure D.1
Basic design of the persistence model.



chemical discharge

transfer of chemical

removal of chemical

C = concentration of chemical ($mg.L^{-1}$)
K = partition coefficient
W = weight of compartment (g)
k_{oi} = reaction rate constant (d^{-1})
transfer rate constants:
k_{12} = suspended solids → water
k_{21} = water → suspended solids ($mg.g^{-1}.d^{-1}$)
k_{13} = sediment → water
k_{31} = water → sediment ($mg.g^{-1}.d^{-1}$)
k_{14} = fish → water
k_{41} = water → fish ($g^{0.2}.d^{-1}$)

where 1 = water, 2 = suspended solids, 3 = sediment, 4 = fish, o = out of the system, i = compartments 1 to 4

Table D.1
Input parameters of the persistence model.[1]

Purpose	Parameter	Status[2]	Purpose	Parameter	Status
System characterization	- month	De	Process description	- hydrolysis rate constant (d^{-1})	M
	- latitude	De		- photodegradation rate constant (d^{-1})	De
	- water temperature (°C)	De		- volatilization rate constant (d^{-1})	De
	- water depth (m)	De		- biodegradation rate constants for	M
	- water volume (L)	De		- biodegradation rate constants for sediment and suspended solids (d^{-1})	M
	- light attenuation in water (low, high)	De		- partition coefficients between water and each compartment	De
	- sediment weight (g)	De			
	- organic content of sediment (%)	De			
	- concentration of suspended solids (ppm)	De		- transfer rate constants between water water and each compartment	De
	- number of fish	De			
	- average fish weight (g)	De			
	- chemical emissions ($mg.d^{-1}$)	De			
Pollutant characterization	- melting point (°C)	M			
	- molecular weight (g)	M			
	- vapour pressure (mm Hg)	M			
	- water solubility ($mg.L^{-1}$)	O-C			
	- octanol-water partition coefficient	O-C			
	- fraction of chemical biodegradable by fish (X)	M			
	- quantum yield and extinction coefficients for 290-400 nm	M			

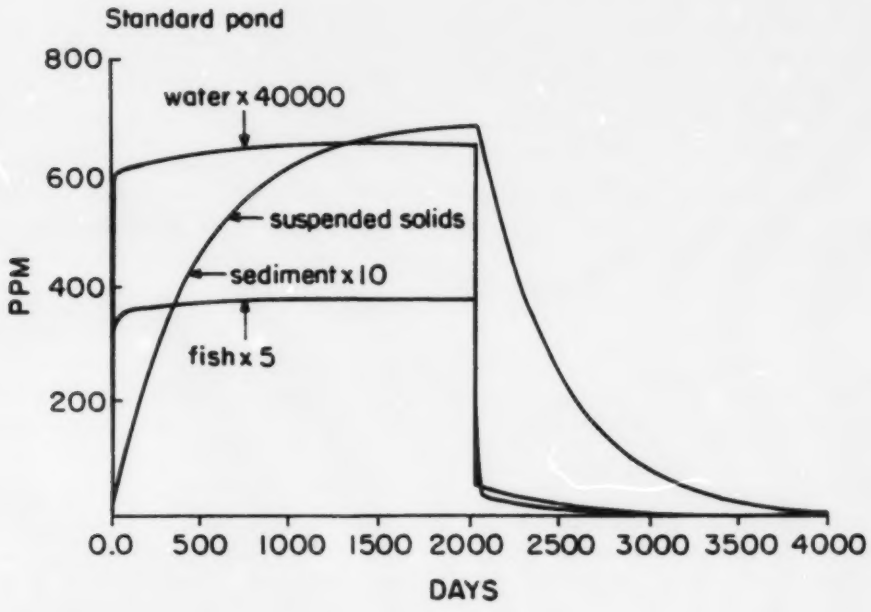
[1] For more detail, see NROC 1981b.
[2] De = Default value – is available within computer program or preferred value can be directly inputted;
M = Mandatory input – necessary for computer analysis;
O-C = Optional Input – conditional – either water solubility or octanol-water partition coefficient must be inputted.

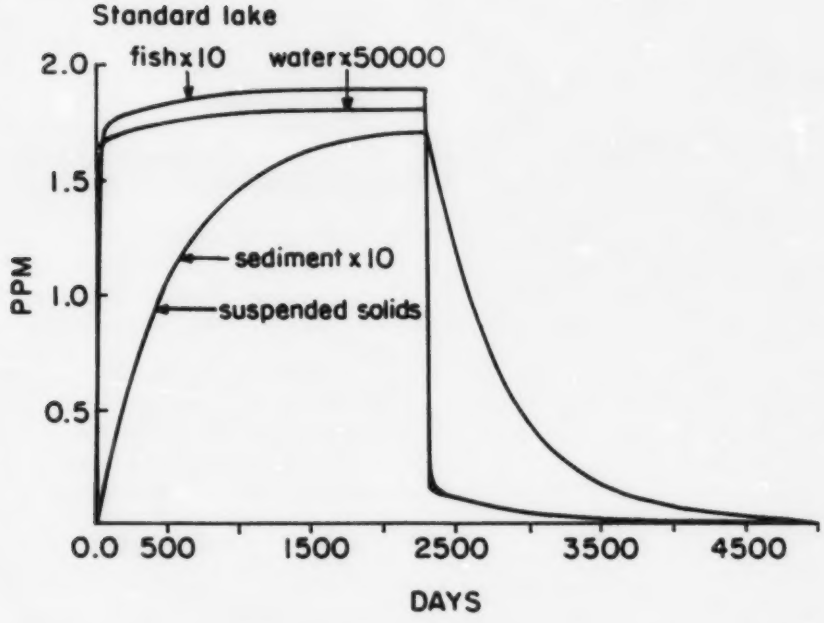
Table D.2
Predicted distribution and degradation routes of hexachlorobenzene at steady state using the persistence model and the standard pond and standard lake system parameters.

System parameter	Standard Pond	Standard Lake
Retentive capacity in system (d)	65.29	60.32
First order half-life in system (d)	45.25	41.81
Fraction of the compound retained in:		
water	0.009	0.059
suspended solids	0.024	0.016
sediment	0.966	0.924
fish	ND[1]	0.002
Fraction of total removal from system due to:		
volatilization	0.929	0.372
photodegradation	0.038	0.609
hydrolysis	ND	ND
degradation in suspended solids	0.001	ND
degradation in sediment	0.032	0.014
degradation in fish	0.001	0.005
Bioconcentration estimate for:		
fish	5 248.07	5 248.07
mollusks	36 372.09	36 372.09
crustacea	3 257.47	3 257.47

[1] Below number of significant figures used in program, ≤ 0.001.

Figure D.2
Accumulation of hexachlorobenzene before, during and after steady state is reached in the compartments of the standard pond and lake of the persistence model





Data Requirements:

Table D.1 represents input to the model in the form of environmental characteristics, physical chemical properties and rate constants for transfer between compartments, and degradation.

Output:

Output is in tabular form for the steady state or fixed solution and in the form of tables or concentration-time curves for various compartments for the dynamic solutions. These are illustrated in Table D.2 and Figure D.2. The overall persistence of the system is also calculated.

Applications:

The model has been applied to the fate of a series of chlorobenzenes from monochlorobenzene to hexachlorobenzene, emitted to water and to other chemicals.

Availability:

Uncertain.

Computer:

Uncertain.

Comments:

This model is of interest because it is virtually the only model of its type generated by the Canadian federal government. Regrettably it appears to have fallen into disuse. It is particularly strong in its treatment of aquatic photolysis. No human exposure is calculated.

Model E

Name:

Environmental Exposure Potentials (EEP)

Type of Model:

Multimedia exposure model.

Reference:

i) Method 503, Draft Compendium of Environmental Exposure Assessment Methods in Chemicals, OECD Chemicals Group and Management Committee, Hazard Assessment Panel (in press 1988).

ii) Klein, W., Kördel, W., Klein, A.W., Kuhnen-Clausen, D., Weiss, M. Systematic approach for environmental hazard ranking of new chemicals, Chemosphere 7:1445-1462, 1988.

Contact:

Prof. Dr. W. Klein, Fraunhofer-Institute fur Umweltchemie und Ökotoxikologie, D-5948 Schmallenberg-Grafschaft, Umweltbundesamt, Bismarckplatz 1, D-1000 Berlin 33.

Description:

EEP is a fugacity-based equilibrium compartmentalization model used by member states of the European Communities to determine the exposure potential of new organic chemicals. The methodology is applied to chemicals being imported or produced in quantities of one tonne per year or more. The assessment depends on a premarketing notification data set, expected use pattern, production volume, physical chemical properties degradation rates and accumulation potential of new chemicals.

The methodology, which is simple, treats multiple or diffuse sources, but does not differentiate between continuous or intermitten emissions.

The model calculates environmental partitioning, quantity in the environment, degradation, and accumulation potential in air, water and soil, employing weighting factors to produce an exposure "fingerprint."

The use patterns of a chemical are broadly classified as: i) intermediate, indicating that a maximum of 3% of production enters the environment; ii) processing, in which 10% is released; and iii) end use, when the whole quantity enters the environment.

Abiotic degradation is not included since it is argued that this implies transformation to another chemical rather than degradation to substances such as CO_2 and H_20.

Scores are developed for each criteria, summed and normalized to permit a standard evaluation.

The exposure fingerprint can be combined with effects data for a total hazard assessment.

Data Requirements:

Data on physical chemical properties of solubility vapour pressure and octanol/water partition coefficient are required as well as classification of use pattern.

Output:

Environmental partitioning is calculated as percent and quantity in air, water and soil; accumulation and biodegradation are also calculated for each of these media. Individual scores are assigned, a total normalised score is calculated and an exposure fingerprint is produced. An example of the input data and scores are given in Table E.1 and exposure fingerprint in Figure E.1.

Applications:

The system is used for each new chemical notified. Results for 25 chemicals have been peer-reviewed and found to be acceptable.

Computer:

EEP runs on an IBM-XT with a DOS operating system and graphics cards. It is written in Turbo Pascal using TURBO.EXTENDER and the Turbo graphix toolbox.

Availability:

Contact Prof. Dr. Klein.

Comments:

This model is relevant because it environmental fate directly. It does not address exposure through contact with various media, although this may be the subject of current investigations. It is also of interest because of its acceptance in the European Community. This German group has been very active and influential in chemical assessments in Europe and must be regarded as leading thinkers in the subject. Their activities are thus worthy of monitoring.

Table E.1
Print-out of input-data and results.

I. S 221-04-01

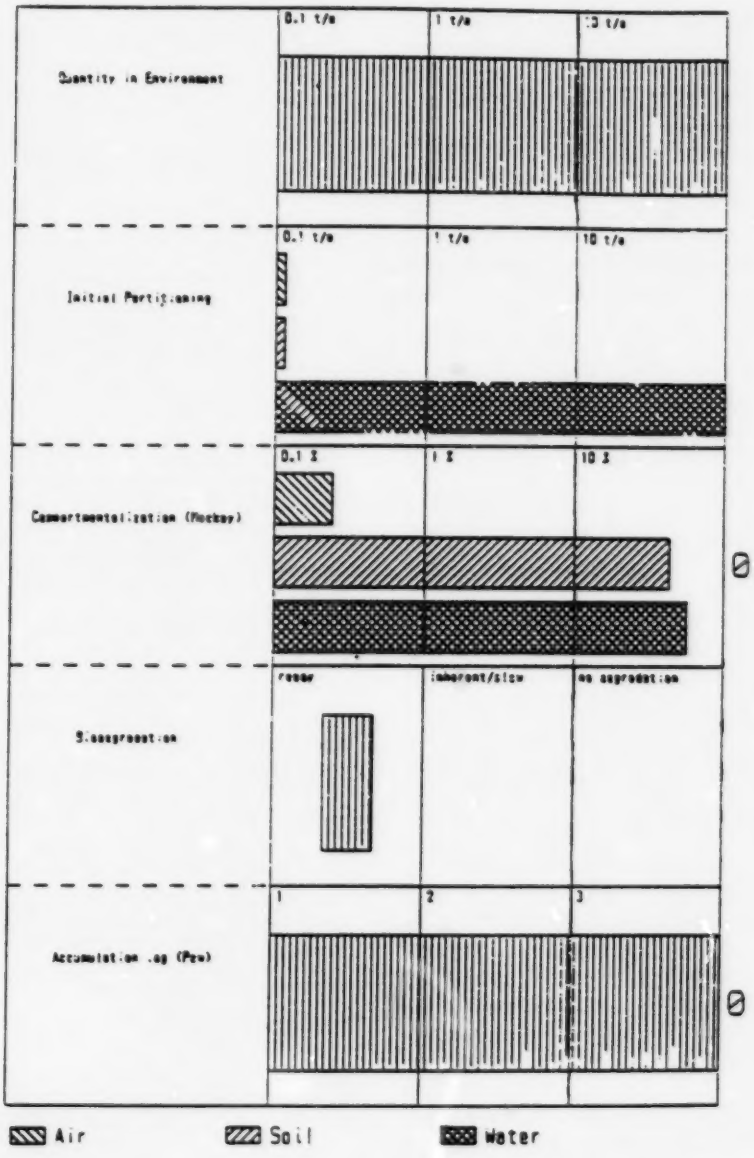
Physicochemical data		
Melting point (K)	: 298.9500	Quality: o.k.
Boiling point (K)	: 649.1000	Quality: Calculated
Density (g/ml)	: 1.113500	Quality: o.k.
Vapour pressure (Pa)	: 0.001210	Quality: o.k.
Water solubility (g/l)	: 0.006150	Quality: o.k.
Partition coefficent octanol/water log (P_{ow})	: 4.540000	Quality: o.k.
Fat solubility (mg/100g)	: 100000.0	Quality: Extrapolated
Surface tension (N/m)	: 0.065000	Quality: o.k.
Degradation data		
Biodegradation	: ready	
Hydrolysis (d)	: 30.000	Quality: o.k.
Photolysis (d)	: No data	
BOD (g/g)	: 1.280000	Quality: o.k.
COD (g/g)	: 2.090000	Quality: o.k.

II. Exposure Results

Partitioning according to Mackay Level 1		
Percentage/tonnage in Air	: 0.24% =	0.24 t/a*
Percentage/tonnage in Soil	: 43.23% =	43.23 t/a
Percentage/tonnage in Water	: 56.53% =	56.53 t/a
Percentage/tonnage in Sediment	: 40.42% =	40.42 t/a
Percentage/tonnage in Biota	: 0.03% =	0.03 t/a
Exposure in Air		
Initial portioning	: 0.00 out of	2.00 scores
Quantity in compartment	: 0.00 out of	4.00 scores
Total exposure	: 0.00 out of	7.00 scores = 0%
Exposure in Soil		
Initial partitioning	: 0.00 out of	2.00 scores
Quantity in compartment	: 4.00 out of	4.00 scores
Accumulation	: 1.00 out of	1.00 scores
Biodegradation	: -2.00 out of	-2.00 scores
Total exposure	: 3.00 out of	7.00 scores = 43%
Exposure in Water		
Initial partitioning	: 2.00 out of	2.00 scores
Quantity in compartment	: 4.00 out of	4.00 scores
Accumulation	: 1.00 out of	1.00 scores
Biodegradation	: -2.00 out of	-2.00 scores
Total exposure	: 5.00 out of	7.00 scores = 71%

* tonne per annum

Figure E.1
Fingerprint of parameters
(exposure substance S 221-04-01)



Model F

Name:
Environmental Partitioning Model (ENPART).

Type of Model:
Multimedia-Compartmental Model.

Reference:
i) Method 505, Draft Compendium of Environmental Exposure Assessment Methods in Chemicals, OECD Chemicals Group and Management Committee, Hazard Assessment Panel (in press 1988).
ii) Environmental Partitioning Model Draft Documentation, Office of Toxic Substances, US EPA, 1982.

Contact:
Exposure Evaluation Division, Office of Toxic Substances (TS-798), US Environmental Protection Agency, 401 M Street, SW, Washington, DC 20460 USA, Attention: Russell S. Kinerson.

Description:
ENPART, developed by the US EPA, provides a first-level screening analysis of chemicals released into the environment. The model is fugacity-based and calculates the steady-state equilibrium concentration ratios between compartments. It identifies dominant pathways and estimates the chemical's persistence and bioconcentration potential. The relative mass distribution is calculated as are transfer and transport rates. The system considers compartments of air, water and soil plus four water subcompartments: sediment, suspended sediments, biota, and ions considered in equilibrium with water. The model is primarily used for chemicals being evaluated for testing.

Data Requirements:
Data on physical chemical properties of solubility, vapour pressure and octanol-water partition coefficients, soil and sediment coefficients are required, as well as environmental information on soil and sediment density, suspended sediment and biota concentrations. Advective flows are not included.

Output:
Output is in the form of concentration ratios between compartments rather than absolute values.

Applications:
The model is used by the US EPA to identify media of accumulation and indicate pertinent tests. Its role in the evaluation of premanufacturing data is not clear.

Computer:
ENPART is written in FORTRAN and runs either on a VAX11/780 or an IBM PC. The IBM PC version is available on a floppy disk.

Availability:
Contact Russell Kinerson.

Comments:
The US EPA has available a number of models and data bases to assist with chemical evaluation in its Washington headquarters. The data provided with their Premanufacturing Notification System is sparse; thus, the methods used are approximate and rely heavily on estimation procedures and personal judgement. As the CEPA requirements are more detailed, the role of models such as this is not entirely clear. There is certainly considerable merit in reviewing US EPA practices.

Model G

Name:
TOXSCREEN.

Type of Model:
Multimedia Model.

Reference:
i) Method 604, Draft Compendium of Environmental Exposure Assessment Methods in Chemicals, OECD Chemicals Group and Management Committee, Hazard Assessment Panel (in press 1988).

ii) Hetrick, D.M., McDowell-Boyer, L.M. User's manual for TOXSCREEN: A multi-media screening level program for assessing the potential fate of chemicals released to the environment. Draft Report. Oak Ridge National Laboratory ORNL/TM-8570. Washington, DC: Office of Pesticides and Toxic Substances, US EPA (Contract No. W-7405-eng-26).

Contact:
Exposure Evaluation Division, Office of Toxic Substances (TS-798), US Environmental Protection Agency, 401 M Street, SW, Washington, DC 20460 USA, Attention: Russell S. Kinerson.

Description:
TOXSCREEN is a time-dependent multimedia screening model used to determine potential for environmental transport and accumulation of chemicals released to air, water or soil. It is expected to identify chemicals that are unlikely to become a problem.

The model is generic in nature and incorporates sophisticated modules for transport in air, water and soil.

Data files contain information on general climatologic and soil data for various regions of the United States. Locations of water bodies and soil relative to sources in the atmosphere must be specified as well as dimensions of the media. An atmospheric point source is assumed to impinge on a water body, if present, at a point immediately downwind from the maximum concentration of the plume.

Atmospheric dispersion downwind from a point source is estimated using a modified Gaussian plume dispersion equation. Chemical migration in soil is estimated by means of the seasonal soil compartment model (SESOIL). Aquatic fate and transport are modelled using the EXAMS model approach. These latter two models were developed by the US EPA office. Dispersion in estuaries and oceans is also incorporated. Interaction between coastal waters and air is not considered.

TOXSCREEN estimates bioaccumulation in aquatic organisms, terrestrial food, animals and plants.

Data Requirements:
The model requires intensive data input including information on characteristics of environment of application and emission sources; chemical and degradation parameters; and climatological, meteorological and hydrological parameters. Data input is dependent on area of application, i.e., estuary, ocean or terrestrial environment.

Output:
An estimation of fate of chemical over a period of time.

Application:
Model has been used for exposure assessment of new and existing chemicals under the Toxic Substances Control Act (TSCA).

Availability:
Contact Russell Kinerson.

Computer:
The code is written in FORTRAN and the model runs on a VAX11/780 computer with a VMS operating system.

Comments:
This is one of the US EPA suite of models mentioned in the comments on Model F.

Model H

Name:

Exposure Commitment Method.

Type of Model:

Exposure Assessment Calculation (not explicitly a model).

Reference:

i) Bennett, B.G. "The exposure commitment method in environmental pollutant assessment." Environ. Monit. and Assessment 1:21-36, 1981.

ii) Bennett, B.G. MARC Reports No. 12, 23. Chelsea College, London, U.K.

Contact:

B.G. Bennett, Monitoring and Assessment Research Centre, Chelsea College, University of London, London, England SW10.

Description:

The exposure commitment method is a time-independent approach for assessing human exposure to environmental pollutants. Essentially, it calculates the cumulative exposure by various pathways for a constant, continuing environmental release. It was originally used by the United Nations Scientific Committee on the Effects of Atomic Radiation (UNSCEAR) to estimate exposure from radio nuclide movement in the environment. It has since been modified for application to organic compounds and metals.

The methodology considers average concentrations in air, water and soil (and other possible media) to perform two assessments: the **exposure** commitment, and the **intake** commitment.

The **exposure** commitment quantifies the intensity and duration of a chemical in the environment and is described by the time integral of concentration, for a specified time, for each environmental compartment. The exposure commitment is thus the area under the concentration-time curve.

The **intake** commitment describes the cumulative intake by a compartment and is described by the time integral of the flux into the compartment.

In the exposure calculations, pollutant transfer factors between compartments are expressed in terms of the ratio of either **exposure** or **intake** commitments for the two compartments or a combination of the two. In equilibrium situations, the transfer factor is equivalent to the ratio of the steady-state concentrations in adjacent compartments.

Exposure or **intake** commitments are calculated sequentially via a succession of compartments for each pathway. Parallel pathways from donor to receptor compartments are considered. For example, exposure might include air inhalation and terrestrial and aquatic ingestion.

Results of each parallel pathway are evaluated and added to give total exposure. This methodology enables the relative contribution of each pathway to total exposure to be assessed. The methodology provides a framework for exposure assessment rather than an actual computer model.

Data Requirements:

The major effort involves synthesis and evaluation of available data. Data requirements, which are not intensive, include information on approximate steady-state concentrations, or environmental levels, over a period of time for various compartments. Where data is lacking, use can be made of observed equilibrium relationships between various compartments. Data may also be required on ingestion and inhalation rates and residence time of the chemical in various media.

Output:

Assessment of relative exposure from each pathway. An assessment of levels of lead in humans and the environment is given in Table H.1.

Applications:

The methodology has been applied to a variety of pollutants, including lead, cadmium, arsenic, nickel, PCBs, and 2,3,7,8-TCDD.

Computer:

Not available in computer code.

Availability:

See contact.

Comments:

This approach is of interest because it has been established for a considerable time and is accepted.

Table H.1
Current levels of lead in the background environment and in humans.

	Air	Diet	Blood
Ingestion pathway	$0.15\ \frac{\mu g}{m^3}$	$40\ \frac{mg}{y}$	$5\ \frac{\mu g}{dl}$
	Direct source to diet	$40\ \frac{mg}{y}$	$5\ \frac{\mu g}{dl}$
Inhalation pathway,	$2\ \frac{\mu g}{m^3}$ urban		$3\ \frac{\mu g}{dl}$
	$0.15\ \frac{\mu g}{m^3}$ rural		$0.3\ \frac{\mu g}{dl}$
		Total	$10\text{–}13\ \frac{\mu g}{dl}$
	Effects level $10\text{–}60\ \frac{\mu g}{dl}$		

Model I

Name:

Preliminary Pollutant Limit Value (PPLV).

Type of Model:

Exposure Assessment Calculation (not explicitly a model).

Reference:

i) Rosenblatt, D.H., Dacre, J.C., Cogley, D.R. "An environmental fate model leading to preliminary pollutant limit values for human health effects," in Environmental Risk Analysis for Chemicals, Ed. R.J. Conway, Van Nostrand Reinhold Co., New York, 1980.

ii) Dacre, J.C., Rosenblatt, D.H., Cogley, D.R. "Preliminary pollutant limit values for human health effects," Environ. Sci. Technol. 14:777-783, 1980.

Contact:

Dr. D.H. Rosenblatt, U.S. Army Biomedical Research and Development Laboratory Bldg. 568, Fort Detrick, Frederick, MD 21701-5010, USA.

Description:

This comprehensive exposure assessment method was developed for the US Army to estimate the allowable level of a pollutant in environmental media by considering human health effects. It is considered to produce a temporary standard, a preliminary pollutant limit value (PPLV), in the absence of any regulatory value. A PPLV or allowable concentration is established for each medium.

Environmental pollutant pathways considered are through air, water, atmospheric vapour and particles to crops, domestic animals and fish. Exposure pathways are identified for each medium; for example, exposure from water may be via fish consumption and water ingestion. Figure I.1 illustrates possible exposure pathways from soil via water.

A single pathway PPLV (SPPPLV) is calculated for each exposure pathway identified in a medium. This SPPPLV is essentially the maximum concentration in the medium that will not produce an unacceptable exposure by that pathway. SPPPLV's for each pathway are normalized to give a single PPLV for the medium considered. The calculation incorporates environmental partitioning characteristics, acceptable daily intake (ADI) and an intake rate. It is assumed that the pollutant is in stepwise equilibrium or steady state from source to receptor. Calculation is usually based on chronic toxicity data, although it can be adapted for sensitive groups. In performing the calculation some judgement must be used and site-specific questions must be considered, for example, whether groundwater is likely to be diluted before it reaches the nearest well. Methodology in evaluating necessary data requires expertise and judgement. A sample calculation is given in Table I.1 with the nomenclature defined in Table I.2.

Data Requirements:

Parameters required include air inhalation and food and water intake rates data on partitioning properties and degradation rates, and chronic effects.

Output:

An allowable pollutant level in each environmental media is calculated.

Applications:

Has been applied to organic compounds (including aldrin, endrin, and toluene), arsenic and mercury.

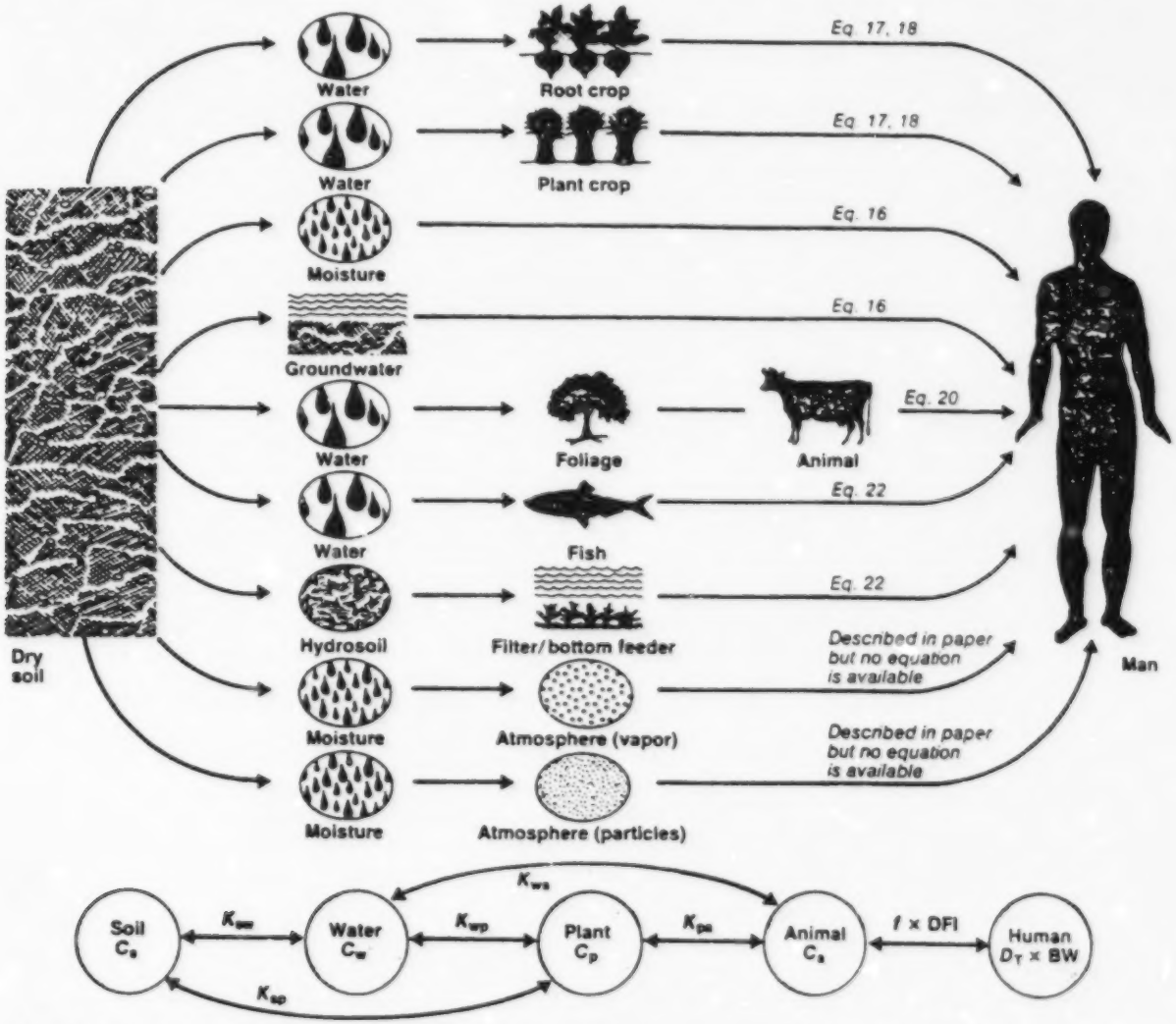
Computer:

Not available in computer code.

Comments:

This was one of the first calculation procedures for human exposure to chemicals in North America. Its focus is to establish clean-up levels or tolerable concentrations, especially in de-commissioned army sites. The author is well respected in this area.

Figure I.1
Pathways from soil via water, plant and animal compartments to humans.*



* In this fate model, the acceptable daily dose of toxicant, D_T, can be obtained from six sources of literature information. The equation for calculating the acceptable daily dose is: $D_T = \frac{f \times DFI \times C_a}{BW} = K_{ps} \times K_{wp} \times K_{sw} \times C_s \times f \times DFI/BW$ (Eq. 2)

Table I.1
PPLV worksheet (with the calculated values for hexachlorobutadiene originating in soil)

Formulas and Calculations	Equation
1. Water Ingestion	
$C_s = 35\ D_T/K_{sw} = 35 \times 5 \times 10^{-7}/(3.84 \times 10^{-3})$	(15-16)
$= 4.6 \times 10^{-3}$ mg kg-1 (SPPLV)	
2. Root Crops	
$C_s = BW \times D_T/(Ksw \times Kwp \times f \times DFI)$	
$= 70 \times 10^{-7}/(3.84 \times 10^{-3} \times 33 \times 0.1 \times 0.63)$	(15-17)
$= 4.4 \times 10^{-5}$ mg kg^{-1} (SPPPLV)	
3. Grain Crops	
$C_s = BW \times D_T/(K_{sw} \times K_{wp} \times f \times DFI)$	(15-17)
(Not Considered)	
4. Meat (by lifetime accumulation, but see text of Section 15-2.4)	
$C_s = BW \times D_T/(K_{sw} \times K_{wp} \times K_{ps} \times f \times DFI)$	
$= 70 \times 5 \times 10^{-7}/(3.84 \times 10^{-3} \times 33 \times 36 \times 0.2 \times 0.63)$	(15-20)
$= 6.09 \times 10^{-5}$ mg kg^{-1} (SPPPLV)	
5. Fish Ingestion	
$C_s = BW \times D_T/(K_{sw} \times K_{wf} \times f \times DFI)$	
$= 70 \times 5 \times 10^{-7}/(3.84 \times 10\text{-}3 \times 1.2 \times 103 \times 0.05 \times 0.63)$	(15-22)
$= 2.41 \times 10^{-4}$ mg kg^{-1} (SPPPLV)	
6. $C_{sa} = 3.78\ D_T$	(15-26)
$= 3.78 \times 5 \times 10^{-7}$	
$= 1.89 \times 10^{-6}$ mg m^{-3}	
$VD_o = 54\ P_o$ (mm Hg) $\times$ MW $= 1.4 \times 10^{4}$ mg m^{-3}	(15-24)
The large ratio of VD_o/C_{sa}, i.e., 7.4×10^{9}, indicates the need for concern over exposure by the vapour route under some conditions.	
7. Normalization	
Only routes 1, 2, 4 and 5 are normalized.	
$C_{sf} = (1/0.0046 + 1/0.0044 + 1/0.0000609 + 1/0.000241)^{-1}$	(15-34)
$= 4.8 \times 10^{-5}$ mg kg^{-1}	
8. Comparison of C_{wf} with C_{wsl}	
$C_{sf} = K_{sw}C_{wf} = 3.84 \times 10^{-3} \times 4.8 \times 10^{-5}$ mg liter^{-1}	(15-33)
$= 1.84 \times 10^{-7}$ mg liter^{-1}	
$C_{wsl} = 4.76$ mg liter^{-1}	
$\therefore C_{wsl} > C_{wf}$, so that solubility is not a limiting consideration	

Table I.2
Symbols and abbreviations involved in the calculations

ADI	=	Acceptable daily intake, mg kg^{-1} day^{-1}
BW	=	Body weight (human), kg
C_a	=	Limiting concentration of pollutant in a food animal, typically cattle, mg kg^{-1}
C_p	=	Limiting concentration of pollutant in a crop used for human or meant-animal food, mg kg^{-1}
C_s	=	Limiting pollutant level in soil for human health effects, mg kg^{-1}
C_{sf}	=	Final C_s value (a PPLV), mg kg^{-1}
C_{si}	=	Initial C_s value (an SPPPLV), mg kg^{-1}
C_w	=	Limiting pollutant level in water for human health effects, mg L^{-1} = mg kg^{-1}
C_{wf}	=	Final C_w value (a PPLV), mg L^{-1} = mg kg^{-1}
C_{wi}	=	Initial C_w value (an SPPPLV), mg L^{-1} = mg kg^{-1}
DFI	=	Daily food intake, kg day^{-1}
D_T	=	Acceptable daily dose of a toxic substance, mg kg^{-1} day^{-1}
f	=	Fraction of total diet represented by food of a given type
K_{ps}	=	C_a/C_p
K_{wp}	=	C_p/C_s
K_{sw}	=	C_w/C_s
K_{ws}	=	C_s/C_w
K_{wf}	=	Concentration in fish/C_w, i.e., bioconcentration factor
K_{ww}	=	C_p/C_w
LD50	=	Single-dose level that kills 50% of a group of test animals of a given species (and preferably strain and sex) with 14-day observation of the animals, mg kg^{-1}
MCL	=	Maximum contaminant level (provisional water limit) in water, mg L^{-1} = mg kg^{-1}
NEL_L	=	Lifetime (chronic) no effect level, mg kg^{-1} day^{-1}
NEL_{90}	=	90-Day (subchronic) no-effect level, mg kg^{-1} day^{-1}
PPLV	=	Preliminary pollutant limit value, mg L^{-1} or mg kg^{-1}
ppm	=	Parts per million (mg L^{-1} in water; mg kg^{-1} in soil, food, or living organisms)
RB	=	Breathing rate, volume of air breathed by a 70-kg human being in 24 hours, m^3 day^{-1}
RB'	=	Breathing rate, volume of air breathed by a 70-kg human being in an 8-hour workday, m^3 day^{-1}
SPPPLV	=	Single-pathway preliminary pollutant limit value, mg L^{-1} or mg kg^{-1}
T	=	Temperature, degrees Kelvin
TLV	=	Threshold limit value for occupational exposure to toxic airborne pollutants over a 40-hour week, mg m^{-3} (or ppm)[a]
W_w	=	Daily water intake, L day^{-1} = kg day^{-1}
[a] mg m^{-3}	=	ppm $\times$ MW/24 at 25°C

Model J

Name:
Fugacity Models.

Type of Model:
Multimedia Exposure Model.

Reference:
Mackay, D., Paterson, S. "Evaluating the regional multimedia fate of organic chemicals: a level III fugacity model", submitted to Environ. Sci. Technol. In press 1990.

Contact:
D. Mackay or S. Paterson, Department of Chemical Engineering, University of Toronto, Toronto, Ontario M5S 1A4, Telephone: D. Mackay - (416) 978-4019; S. Paterson - (416) 978-5873.

Description:
In the last decade, a series of models has been developed at the University of Toronto by Mackay, Paterson and coworkers. They include simple (level I) models describing the fate of conservative chemicals at equilibrium; level II models, which include reaction and advection; level III models, which treat intermedia transport at steady state; and level IV models, which treat time-varying conditions. Most relevant to the present discussion is a recent level III model developed for the Ontario Ministry of the Environment.

This fugacity-based multimedia environmental model treats four bulk compartments: air, water, soil and sediment. Each bulk phase is considered to consist of subcompartments of varying fractions of air, water and organic matter. Equilibrium is assumed to exist within but not between compartments.

The algebraic model solution incorporates expressions for emissions, diffusive and non-diffusive transfer processes, advective flows and degrading reactions.

The model calculates the steady-state distribution of a chemical and its persistence in the environment. Media of accumulation and dominant pathways of transfer are determined. The resulting predicted environmental concentrations can be combined with air inhalation and water and food ingestion rates for a preliminary estimate of human exposure.

Partitioning of chemical between phases is expressed in terms of the equilibrium criterion of fugacity. Fugacity can be considered a surrogate for concentration and is related to concentration through a fugacity capacity or Z value. These Z values are calculated from a chemical's physical properties of molecular weight, vapour pressure, solubility and octanol-water partition coefficient, as well as properties of density and fraction organic content of the phase into which it partitions.

These Z values, which are equivalent to half a partition coefficient, characterize a phase independently.

Diffusive transfer between air and water, air and soil, and water and sediment is estimated from mass transfer coefficients, interfacial areas, diffusivities and path length.

Non-diffusive processes include wet and dry atmospheric deposition, leaching from groundwater, sediment deposition, burial and resuspension and runoff from soil, and are estimated from a flow rate, Z value and fugacity.

Degradation in each compartment or subcompartment is included by means of a rate constant.

The model equations incorporate expressions for advective flow of chemical into and from a region. Emissions of chemical to each phase must be quantified.

Four mass balance equations representing the four bulk phases are solved in terms of fugacity. Concentrations and amounts are estimated for the bulk phases. Fugacities of subcompartments are set equal to those of the bulk phase. Thus, concentrations and amounts in subcompartments are readily calculated.

Data Requirements:
Data requirements include a minimum set of regional environmental characteristics, including volumetric dimensions, relative proportions of fluid, gas and solid in each phase, densities, and fraction organic content; chemical emission rates; physical chemical properties of vapour pressure, solubility and octanol-water partition coefficient; and chemical reactivity in the form of rate constants.

Output:
Output from the model includes input chemical properties, reaction rate constants, emission rates, any background (advective inflow) concentrations and dimensions, and properties of all bulk and subcompartments. Concentrations, amounts and fugacities are provided for each phase and subphase. Transfer and transformation rates are given for individual and combined processes and a total mass balance is assembled.

Applications:
The model has been applied to PCBs, benzene, hexachlorobenzene, benzo(a)pyrene, mirex and trichloroethylene in the southern Ontario region. The results illustrated in Table J.1 are in order of magnitude agreement with available reported data. The model is believed to be useful in predicting the environmental fate and human exposure to persistent organic chemicals which are released more-or-less continuously into the environment.

Computer:
Available on a floppy disk for IBM-PC.

Availability:
Can be purchased on a cost-recovery basis from D. Mackay or S. Paterson, at the University of Toronto, for $30.00.

Comments:
This model is probably the most advanced environmental fate model developed for Canadian conditions. It has been extended recently to include assessment of human exposure, but no publications are yet available, although the general principles have been described in a chapter in "Carcinogen Risk Assessment," edited by Travis.

Table J.1
Calculated and reported concentrations for the four bulk phases and fish and bulk phase fugacities

Compound	Air (ng/m3)		Water (ng/L)		Soil (mg/kg)		Sediment (ng/g)		Fish (mg/kg)		Bulk Phase Fugacities (Pa)			
	calculated	reported	calculated	reported	calculated	reported	calculated	reported	calculated	reported	Air	Water	Soil	Sediment
6-CB	1.4	1-10 (28)	5	1-10 (28)	.04	.01-.02 (28)	80	10-100 (28)	2	N.D.-1.7 (28)	$7.8x10^{-9}$	$8.7x10^{-8}$	$1.4x10^{-7}$	$2.2x10^{-7}$
benzene	2500	16000 (29) (N.D.-380000)	290	<100000 (29)	.00001	-	0.5	-	.002	-	$8.0x10^{-5}$	0.0021	$6.0x10^{-5}$	0.0021
BAP	3.0	1.32 (29) 7.1 (22) 4.7 (23)	11	28.2 (23)	.04	.1 (29) .1 (22) .3-.5 (23)	190	80-300 (29)	0.26	.14 (29)	$1.8x10^{-10}$	$1.1x10^{-9}$	$1.1x10^{-9}$	$4.5x10^{-9}$
HCB	.2	.2 (26)	1.3	.05-1 (29)	.0009	-	7	3-100 (29)	.01	.05 (30) .003 (31)	$1.9x10^{-9}$	$2.8x10^{-7}$	$1.4x10^{-7}$	$9.2x10^{-7}$
mirex	.0001	-	.002	.002 (32) 30 (29) <1 (33)	$8x10^{-6}$	-	.07	20 (29) 69 (34)	.0001	.003 (30) N.D.-.04 (29)	$2.5x10^{-13}$	$4.3x10^{-10}$	$3.8x10^{-10}$	$2.1x10^{-9}$
TCE	11000	6400 (27)	270	<6000 (27)	$3.7x10^{-5}$	-	0.6	.07 (27)	0.0026	0.0001-0.01	0.00021	0.0025	0.00021	0.0025

Model K

Name:
SIMPLESAL.

Type of Model:
Multimedia-Compartmental Model.

Reference:
Method 506, Draft Compendium of Environmental Exposure Assessment Methods in Chemicals, OECD Chemicals Group and Management Committee, Hazard Assessment Panel (in press 1988).

Contact:
D. van de Meent, National Institute of Public Health & Environmental Hygiene (RIVM), P.O. Box 1, 3720 BA Bilthoven, The Netherlands, Telephone: 030-743130.

Description:
SIMPLESAL is a spreadsheet-based, multimedia, fugacity compartmental model, which can be used to estimate steady-state or time-dependent concentrations of organic compounds as well as heavy metals. The model, which determines dominant environmental pathways and processes for micropollutants, was designed as a screening tool to predict results of various scenarios for emission control of new and existing chemicals. It considers compartments of air, water, suspended solids, aquatic biota, sediment and soil.

SIMPLESAL incorporates four modules for solving a simultaneous set of either algebraic (steady-state) or differential (unsteady-state) equations:

i) a pre-processor unit to convert input data in environmental and physicochemical properties into mass balance equations;

ii) matrix inversion subroutine to calculate steady state concentrations from a set of algebraic equations;

iii) a numerical integration subroutine to calculate dynamic concentrations; and

iv) a graphics package to display output.

The following processes, illustrated in Figure K.1, are included:

i) advective flows in air, water and suspended matter;

ii) diffusive transfer between air-water, air-soil, and sediment-water;

iii) wet and dry atmospheric deposition, sediment deposition, resuspension and burial;

iv) bioconcentration in aquatic biota;

v) leaching from soil to groundwater;

vi) degradation by biotic and abiotic transformation.

Data Requirements:
Data requirements include dimensions and properties of, and emission rates into, various media; air and water residence times; parameters for intercompartment transfer in association with particulates; physico-chemical properties of water solubility, vapour pressure and octanol-water partition coefficient; and degradation rate constants for biotic and abiotic transformation.

Output:
The output is in the form of either steady state environmental concentrations or dynamic response to changing emissions, as well as intercompartment transfer rates, transformation rates and advective flow rates.

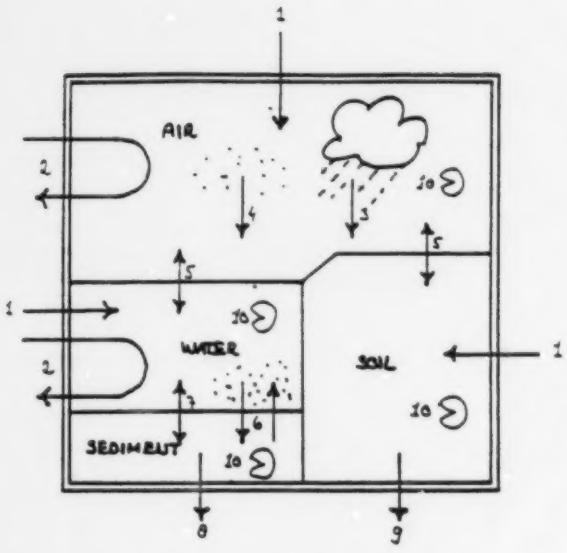
Applications:
The model has been applied successfully to proposed environmental management of benzene, cadmium, lindane and copper in the Netherlands.

Computer:
The steady-state version of the model runs on an IBM-PC compatible computer using a Lotus 1-2-3 spreadsheet. The dynamic version requires a Turbo-Pascal™ compiler and a dynamic simulation program, FRAME, which is available on floppy disk.

Availability:
Not known, but probably freely available on request.

Comments:
This is a fugacity model applied to conditions existing in the Netherlands. It is quite similar in principle to the Canadian fugacity models.

Figure K.1
SIMPLESAL processes.



Processes included in SIMPLESAL:
Emissions to air, water and soil (1); advective import in and export from air and water (2); air-water and air-soil exchange through wet deposition (3), dry deposition of aerosol-particles (4) and gas-exchange (5); water-sediment exchange through sedimentation and resuspension of particulate matter (6) and direct exchange (7); sediment burial (8); soil leaching (9); abiotic and biotic degradation (10).

Model L

Name:
Aid for Evaluating the Redevelopment of Industrial Sites (AERIS).

Type of Model:
Multimedia Risk Assessment Model (that runs within an expert system programming environment).

Reference:
Contaminated Soil Cleanup in Canada – Volume 2: Development of the AERIS Model (Interim Report); scheduled to be superseded by Volume 5 in mid-1989.

Contact:
Brett Ibbotson, SENES Consultants Limited (416) 764-9386 or Art Stelzig Industrial Programs Branch, Environment Canada (613) 953-1134.

Description:
AERIS uses environmental and toxicological information to estimate exposures (and therefore risks) that site users or visitors can receive as a result of contaminants present in soil. For sites where redevelopment is being considered or proposed, the exposure estimates can be used to determine soil clean-up guidelines. Innovative aspects of AERIS are that information about the contaminant, the site user, and the local environment are assembled in a user-friendly, expert system programming environment and integrated to provide a consistent approach to establishing soil guidelines.

AERIS consists of four basic elements: an "intelligent" preprocessor, a set of component modules, a postprocessor, and supporting data base. The preprocessor is a series of easy-to-understand questions that AERIS asks the model user about the redevelopment scenario to be evaluated. The user can either answer with site-specific information accept default values that the model suggests. If the user is uncertain as to how to respond to a specific question, additional explanation or assistance can be shown on-screen. The preprocessor is referred to as intelligent because it incorporates expert system technology. It uses a set of rules to decide when sufficient information has been provided, to aid the user to estimate unknown input parameters, to check for errors in the answers as they are being provided, and to control the flow of information among other elements of AERIS.

The preprocessor passes the information about the redevelopment scenario provided by the user to the component modules. The modules consist of equations that estimate pseudo-steady state concentrations of the contaminant in environmental compartments (such as air and ground water) on the basis of the concentration of the contaminant in soil. The predicted environmental concentrations are subsequently used to estimate the doses incurred by a site user from a specific pathways such as breathing air or drinking ground water. The doses from the individual pathways are combined to estimate the total dose, which, in turn, can be compared to a total dose

that toxicological information indicates is "acceptable." The acceptable concentration in soil for a contaminant is the concentration that produces a dose equal to but not greater than the acceptable dose.

Input Model Requirements:

This is influenced by the scenario being evaluated. Default values or on-screen assistance in providing inputs are offered throughout the program. Basic input requirements include physico-chemical and toxicological information about the contaminant of interest, intended future use of the site, physical and behavioral characteristics of the receptor (site user), site meteorology, characteristics of the soil and the underlying formation, and ground water regime.

Output:

All of the estimated environmental concentrations, the doses for each pathway, and the total dose estimates are passed to the postprocessor, which offers the user various tabular and graphical ways to display the results.

Applications:

The lack of precedent in establishing soil guidelines, the mandate of regulators and decision makers to safeguard the public, the growing recognition of site owners and potential owners to understand the liabilities that a site may pose, result in various situations to which AERIS could be applied.

i) AERIS could be used by regulatory agencies asked to comment on the acceptability of a contaminated site for a proposed use, to determine whether clean-up efforts are necessary, or identify clean-up objectives.

ii) AERIS could be used by current owners or prospective buyers of sites interested in knowing whether remedial action may be necessary, and if so, to what extent. For contaminants that have not been addressed by regulators, AERIS could be used to give a first approximation of clean-up guidelines that eventually may be established.

iii) AERIS could be used by educators to demonstrate to students the interrelationships between environment and dose and as a means for incorporating risk assessment into decision-making processes.

Hardware Requirements:

AERIS is designed to run on the IBM Personal Computer (TM), IBM XT (TM), IBM AT (TM), IBM Personal System/2 (TM), and compatibles. Minimum requirements include:

i) a single double-sided floppy disk drive or hard disk

ii) a minimum of 256K bytes of RAM

iii) PC-DOS/MS-DOS operating system, version 2.0 or higher

iv) math co-processor

Availability:

Not yet available to the public. Inquiries should be directed to Environment Canada or SENES Consultants Limited as noted above.

Comments:

AERIS is not a comprehensive multi-media model since it considers only phases of air, soil and groundwater. However, the use of an expert system to aid the user is innovative and worth noting.

Model M

Type of Model:
Multimedia-Compartmental Model (MCM).

Reference:
i) Cohen, Y., Ryan, P.A. "Multimedia modelling of environmental transport: trichloroethylene test case," Environ. Sci. Technol. 19:412-417, 1985.
ii) Ryan, P.A., Cohen, Y. "Multimedia transport of particle-bound organics: benzo(a)pyrene test case", Chemosphere 15:21-47, 1986.

Contact:
Dr. Y. Cohen, National Center for Intermedia Transport Research, University of California, Los Angeles, CA 90024, USA, Telephone:

Description:
The US Environmental Protection Agency has funded about ten centres to study specific environmental issues, such as groundwater or ecosystems. One of these centres, the NCITR at UCLA, is under the direction of Dr. Y. Cohen. It has built on a particular expertise in air pollution, especially dry deposition of aerosols, and has developed several models and modelling approaches especially directed to contaminants transported by air. The studies discussed below are examples of the centre's output, but its other active programs in this area should be monitored closely.

This multimedia model describes the dynamic distribution of organic pollutants in a six- compartment system, consisting of air, water, soil, sediment, suspended sediment and biota.

It incorporates diffusive and non-diffusive transfer processes, advective and convective flows, and first order reactions in various compartments. In the case of air advection, a factor for atmospheric recirculation is included, which increases the residence time of air. It can be applied to both particulate-bound and non-aerosol pollutants. Processes of washout by rain and dry deposition are quantified. The model solution of a set of six differential equations produces a concentration-time profile for each compartment.

Data Requirements:
As in the case of other multimedia-compartmental models, input data is required in the form of environmental media properties, physicochemical and thermodynamic properties of the chemical, partition and transport coefficients, climatic conditions and initial background concentration or emission data.

Applications:
The model has been applied to evaluate the fate of trichlorethylene and produced reasonable agreement with available data. It has also been successfully applied to the dynamic distribution of benzo(a)pyrene in southeast Ohio. In the second study, the fate of benzo(a)pyrene in air, water and soil was explored for steady and varying emissions.

Computer:
Generally mainframe.

Availability:
Probably freely available on request.

Comments:
No packaged documented models are as yet available from this group, although such models may be produced in the near future. The models will probably reflect air-soil situations, with few aquatic components, as is found in dry California conditions.

3. Critical Evaluation

3.1 Summary Spreadsheet

Table 3.1 is a summary spreadsheet of the models and their characteristics. It is clear that there is a wide diversity of model types. The most comprehensive models are the GEOTOX and TOXSCREEN systems, the latter being really a compilation of several modular models. All the essential processes of interest to H&W have been treated in at least one model. Thus, the component parts of a model suitable for H&W exist, but are not yet integrated into a single working system.

It is possible to examine in great detail the model-by-model treatment of specific processes such as fish-water bioconcentration or inhalation. This detailed examination is best delayed, however, until it is decided which model (or models or model components) will be used. Fortunately, this examination is not difficult, since it involves obtaining the advice of experts in the various areas.

We offer the following comments in this area:

1. A major weakness of all modelling efforts is the lack of discharge or source data, i.e., kg/year of chemical discharged. Under CEPA this situation (which is not the fault of the model) should be improved.
2. The environmental fate models differ greatly in complexity. The simplest tend to be steady-state fugacity models, and the more complex are concentration expressions in differential equation form. After the initial intellectual commitment to understand the fugacity concept, its use on a routine basis is easier.
3. Major weaknesses still exist in the areas of:
   soil ingestion
   plant uptake from soil and air
   sediment-water exchange
   inclusion of indoor exposure
   inclusion of occupational exposure
   treatment of imported vs locally grown food
   dermal exposure
   extreme lifestyle characterization
   gastro-intestinal uptake
   human metabolism
4. Several models, notably RAPS and GEOTOX, have characterization of human exposure uptakes. The Stevens/Wisconsin dioxin approach to the human on consumption of vegetation and dairy products is very good. EPA reports also address this issue very thoroughly. The AERIS approach is superior for the soil to human route.

Recent experience has shown that models can play an invaluable role in suggesting strategies for reducing levels of human contamination and getting rid of sources of contamination. They can provide guidance for monitoring programs both before and after remedial activities. It is now possible to calculate the entire sequence of events from chemical emission to dispersal in the environment, uptake in foodstuffs, human consumption, and concentration in human tissues. Charting the sequence is a long and difficult process containing many difficult calculations, but it is possible. It is very encouraging that in cases such as dioxins this calculation has been completed and the human tissue concentrations observed have been matched with those calculated. This has lent confidence to the use of models. There is a need to include in exposure assessments the possibility that low amounts of chemical may reach the human receptor by unexpected routes. At very low environmental concentrations these normally ignored routes can become important, for example, the inhalation of trihalomethanes showering, and the transfer of dioxins from paper to food.

Only the EPA models adequately examine food preparation and drinking water treatment as methods of reducing exposure. It is not entirely clear how this is best done, or even if it should be done. An argument can be made that it is *potential* exposure that is of concern, not necessarily *actual* exposure.

Table 3.1
Summary Spreadsheet of the Models and their Characteristics

Category		GEOTOX	RAPS	MNSEM	Persistence	EEP	ENPART	TOX-SCREEN	Exposure Commit-ment	PPLV	Fugacity	SIMPLE-SAL	NCITR	AERIS
Compartment														
Air	- bulk	N	Y	Y	N	Y	Y	Y	N	N	Y	Y	Y	Y
	- vapour	Y									Y			
	- partic.	Y									Y			
Water	- bulk	N	Y	Y	Y	Y	Y	Y	N	N	Y	Y	Y	Y
	- water	Y			Y						Y			
	- fish	Y			Y		Y	Y			Y			
	- shellfish				N						N			
	- susp. sed.	Y			Y		Y				Y			
Soil	- bulk	Y	Y	Y	Y	Y	Y	Y	N	N	Y	Y	Y	Y
	- solids										Y			
	- air										Y			
	- water										Y			
	- unsat. zone	Y									N			
	- sat. zone	Y									N			
Sediment	- bulk	Y	Y	Y	Y	N	Y	N	N	N	Y	Y	N	N
	- solids										Y			
	- porewater										Y			
Groundwater		Y	Y	N	N	N	N	Y	N	N	N	N	N	N
Vegetation		Y		N	N	N	N	Y	N	N	N	N	N	Y
Transfer processes														
Diffusive Transfer		Y	Y	Y	Y	Y	Y	Y	N	N	Y	Y	Y	Y
	- air/soil	Y	N	Y	N	Y	Y				Y	Y	Y	Y
	- air/water	Y	N	Y	N	Y	Y				Y	Y	Y	Y
	- sed./water	Y	N	Y	Y	N	Y				Y	Y		N
Non-diffusive Transfer		Y		N	N	N	N	Y	N	N	Y	Y	Y	N
	- rain washout	Y	Y								Y	Y	Y	
	- wet depos'n	Y	Y								Y	Y	Y	
	- dry depos'n	Y	Y								Y	Y	Y	
	- soil runoff	Y	Y								Y	N		
	- leaching	Y	Y								Y	N		
	- susp. sed. resuspn	Y	N								Y	Y		
	- sed. burial	Y	N								Y	Y		

Tab le 3.1 (cont'd)

Category	Geotox	RAPS	MNSEM	Persistence	EEP	Enpart	Commit-Toxscreen	Exposure ment	PPLV	Fugacity	Simplesal	NCITR	AERIS
Advective Flows													
In	N	N	N	N	N	N	Y	N	N	Y	Y	Y	N
Out	Y	N	N	N	N	N	Y	N	N	Y	Y	Y	N
Degradation								N	N				
Biotic	Y	N	Y	Y	Y	N				Y	Y	Y	N
Abiotic	Y	N	Y	Y	N	N	Y			Y	Y	Y	N
NATURE OF MODEL													
Steady	Y	Y	Y	Y	Y	Y	Y			Y	Y	Y	Y
Unsteady	Y		N	Y	N	N	Y			Y	Y	Y	N
EXPOSURE PATHWAYS	Y	Y	N	N	N	N	N	Y	Y	Y	N	N	Y
Inhalation of Air								Y	Y				
- atmospheric	Y	Y								Y			Y
- showers	N	Y								N			N
Ingestion of water								Y	Y				
- drinking	Y	Y								Y			Y
- bathing	N	Y								N			N
- swimming	N	Y								N			N
Ingestion of food													
- fish	Y	Y						Y	Y	Y			N
- shellfish	N	Y								N			N
- crops	Y	Y						Y	Y	Y			Y
- domestic animals	Y	Y						Y	Y	Y			N
Accidental Ingestion of Soil and Water	Y	Y								N			Y
Dermal Absorption	Y	Y								N			N
Other Activities	N	Y								N			N

3.2 Are These Models Suitable for Use Under CEPA?

In this evaluation we proceed by asking and answering, a series of questions of the spreadsheet.

Could one of the existing models be adopted for immediate use?

The obvious answer is no. Neither of the prime candidates, TOXSCREEN and GEOTOX, is designed for Canadian conditions. Fugacity, when its exposure component is complete, will be a candidate.

Could one of these models be modified?

Only TOXSCREEN, GEOTOX and the fugacity models are suitable.

TOXSCREEN is a very large, complex assembly of several detailed process models. Understanding the entire system would be a formidable intellectual challenge. It is not certain that it could be made available. Most importantly, it relies on geographic data (hydrology, meteorology, census regions, etc.) gathered from agencies such as the US Geological Survey and the US Weather Service. Although similar groups exist in Canada, the available landscape data is in a quite different form and extensive program modification would be required. To retrieve and modify TOXSCREEN for Canadian conditions would require a substantial effort, mainly in the environmental area for exposure estimation.

GEOTOX is more promising. It too is a large, complex model fully understood only by its developers (principally Dr. Tom McKone). The principal modifications would be to the landscape data which is entirely US-oriented. It may be weak in treating areas with substantial water body influence such as the Great Lakes Basin and maritime areas, especially on the east coast. It could be obtained and modified by contract and licensing agreement from the developers.

The fugacity model, discussed later, is complete for environmental fate assessment but is not yet complete for comprehensive exposure evaluation.

In summary, modification of one of these existing US models is technically feasible, but would require allocation of considerable resources, especially in the environmental area.

Table 3.2 appended to this report is a summary of equations used in US EPA models.

Could one of the existing models be adopted and expanded to meet H&W needs?

There are several possibilities. An attractive option would be to build onto one of the existing simple environmental exposure models specific Canadian human exposure conditions of food and water consumption. If it is desired to minimize effort devoted to environmental modelling, as is the approach in various European countries and Japan a "custom" exposure module could be added. Modifying and expanding is not very difficult from starting from scratch but using existing modules.

In our judgement, the best option is to develop a model specifically for Canadian conditions by adopting the best features of existing models. This would allow for some of the excellent process expressions in models such as RAPS, AERIS, GEOTOX and TOXSCREEN, to be used but in a different context.

At this point it is useful to digress to address the issue of what type of model is needed. Ultimately this is a policy matter for the Department, but we offer the following comments for consideration.

3.3 What Type of Model is Needed?

First it is advisable to clarify how modellers view their efforts. Often there are strong misconceptions and over-expectations about the nature of models, what they can accomplish, and how accurately they will do it.

3.3.1 The Nature of Models

Models are best regarded only as *aids* to the assessment of chemical behaviour. They help overcome our inherent mental inability to store and manipulate large amounts of data, and allow us to estimate environmental and exposure phenomena quantitatively. But just as a variety of modes of transportation (such as plane, car, boat and bicycle) help us get from place to place, so can a variety of models serve different purposes. Some are steady state, some unsteady state, some regional, some evaluative, some very simple, and others very complex. This is regarded by modellers as a healthy state of affairs: the user has the benefit of a variety of models.

A frequent problem is lack of care in model selection. Disappointment can result if the model selected is not appropriate for the task. The key first step is to formulate properly the question to be answered by the model. Models and modellers fall into disrepute when models are used in attempts to answer questions for which they are fundamentally ill-designed.

A strong case can be made for using the simplest available model. This is not a new sentiment. There is much concern in modelling circles that the increasing availability of complex models is an invitation to abuse when unskilled individuals inadvertently misuse the models and misinterpret the results. Perhaps just as the authority to drive a car or remove a person's appendix is vested only in individuals who have gone through some training program, the privilege of using models for regulatory purposes should require some training. At present, the need for such a training requirement has not been acknowledged.

The model results and the quantitative conclusions should be easily interpretable preferably verifiable in a relatively simple "back of an envelope" calculation. A major role of the model is to sort out the important processes from the many interacting processes which occur in the environment and in humans. Once the key processes are identified, it is often easy to conduct relatively simple calculations of, for example, concentration or persistence and to deduce the dominant behaviour of the chemical. It is highly desirable that the user perform such post-modelling evaluations. A more detailed analysis can then be made of those processes which comprise the dominant exposure route, e.g., water-fish-ingestion as food.

3.3.2 Canadian Regulatory Considerations

It is not clear to the authors how H&W and DOE will eventually address the task of modelling under CEPA, but it is obvious that H&W will not be inclined (nor is mandated) to undertake extensive environmental distribution calculations. Obviously a joint, integrated effort is needed, with common objectives and expectations.

One approach would be for H&W to adopt a fairly simple, robust environmental fate model similar to those used by OECD and build on it a Canadian exposure assessment. DOE could then modify and expand the fate model to satisfy its own needs. In our opinion, it could be unwise for H&W to wait for DOE to develop a fate model, as this could delay the entire process. To get the process started, it would be useful to have even a "straw man" fate model – that is, a model that demands the available input data and generates the required output data using the best and most available model expressions, but not necessarily fully validated or justifiable expressions. Even if the results are fairly inaccurate, the process of modelling will at least be started. With relatively little effort, one of the existing fate models could be applied to Canadian conditions.

The effect of international trade changes (e.g., GATT, US-Canada Free Trade) on chemical assessment needs and requirements and mutual acceptability of foreign assessments is not clear. There is a trend for "harmonization," but there is a slowness in the US towards harmonization, with OECD for example. How Canada will fare in this context as a strong trading partner with the US is uncertain.

It is noteworthy that the US EPA has devoted many millions of dollars to model development in recent years. A case can be made for obtaining the opinion and exploiting the experiences of the US EPA on both regulatory and scientific levels. The information gained is freely available to the Department and should be exploited. Close liaison is also desirable with some provinces, particularly Ontario, which are active in this area.

3.3.3 Canadian Geographic Considerations

Canadian conditions are quite different from those of other countries:

(a) The area is very large and the average population density very low, typically 1/10th that of the US and 1/100th that of industrialized Europe. But there are areas of very high population density and industrial activity along the Canada-US border.

(b) Because temperatures are generally lower than are experienced elsewhere, the partitioning characteristics of chemicals are fundamentally different from those applying in warmer climates. Notable is the "toxic cold finger" effect, which causes high PCB levels in lipids in Arctic animals.

(c) An important part of the Canadian identity is the national perception of a polar, cold, near-pristine country, still populated by the native peoples, with unique wildlife and relatively unspoiled areas for fishing and hunting. Preservation of these features is important to Canadians, thus there is a uniquely peculiarly Canadian need to understand how chemicals will affect the northern ecosystem. A strong case can be made for including a specific "cold climate" assessment, which would study the unusual lifestyles and food consumption patterns of northern residents.

(d) There is a heavy reliance on imported fruits and vegetables from more southerly regions with better growing climates.

(e) There is a strong influence of advected (carried by air and water currents) contamination from the US. Acid rain is the most notable form but there is appreciable import of other chemicals. This is not the case in regions such as California which receives relatively pristine Pacific advection.

(f) There are intense regional differences in ecosystem or ecotome type across the country which makes evaluation of chemicals on a national basis very difficult. To illustrate this Figure 3.1 is a map of Canada divided into five regions which could be considered for separate evaluation. These are:

1 - Pacific coast and mountains
2 - Southern prairies
3 - Great Lakes, St. Lawrence Basin
4 - Maritimes
5 - Northern regions

These do not follow political boundaries. Consideration of the differing climates, terrains, lifestyles and wildlife in these regions suggests that to lump them together could be very misleading. They have quite different landscapes, populations and industrial activities. Human exposure to chemicals is thus likely to be quite different from region to region.

3.3.4 Fugacity and Concentration Models

Several jurisdictions in Europe and North America have adopted and adapted the fugacity modelling approach developed by the authors of this report at the University of Toronto under a grant from the US EPA. Ultimately, fugacity and concentration models should yield similar, even identical, results. Most environmental and human exposure scientists are more familiar and comfortable with concentration units, although there is increasing use of fugacity, especially in Germany, the Netherlands and Japan. Obviously the authors of this report are not impartial in this area. We advocate the use of fugacity models for the following reasons:

(a) There is widespread use in other jurisdictions.

(b) Successful fugacity models have already been developed for parts of Canada (Ontario and parts of the Great Lakes Basin).

(c) The application of the fugacity concept to environmental modelling is a Canadian development.

(d) There exist fugacity models for key processes, including bioconcentration, and human pharmacokinetics.

(e) Work is well advanced on fugacity models for plant uptake of chemicals from soil and air. It is believed that these models are the most advanced of their type.

(f) There is considerable local experience in fugacity modelling.

A frequently considered option allowing for individual creativity is to assign the task of model development to more than one group. The efforts are then brought together and

reviewed and the best approach, or a hybrid approach is adapted. This was recently done successfully by the International Joint Commission.

3.4 What Should Health & Welfare Canada Do?

We understand that H&W has taken into consideration the factors listed above and has developed a policy towards modelling including resolution of the human and financial resources (in house and contracted out) which will be devoted to this task. The resources will largely dictate the extent of the effort and the complexity of the models. Some key issues are:

- role of DOE
- availability of models to public and industry
- time available for assessments
- regional considerations
- complexity of model
- how models can be best updated and how frequently

A Suggested Course of Action

We suggest the following:

(a) H&W should adopt relatively simple environmental fate models similar to those used in European countries. This could be done by a relatively modest contract. The models should treat separately at least the five regions named earlier.

(b) H&W should build on to these models (either in house or by contract) human exposure models by exploiting available information on population and lifestyle. Because of differing habits, this treatment should separate age classes: infant, child, adolescent and adult.

(c) Close liaison and peer review should be sought with other modellers, especially in the US and Europe, to ensure that Canadian modelling approaches reflect the current state of the art.

Model intercalibration exercises would be particularly valuable to ensure that assessments made by different systems in other jurisdictions are yielding results which are similar or explicably different. For example, a common set of physical chemical properties and use characteristics could be defined for selected chemicals X, Y and Z and the chemicals could be assessed independently by the various groups. When the results are compared, they should be broadly similar. It is the same "round robin" principle used in chemical analyses.

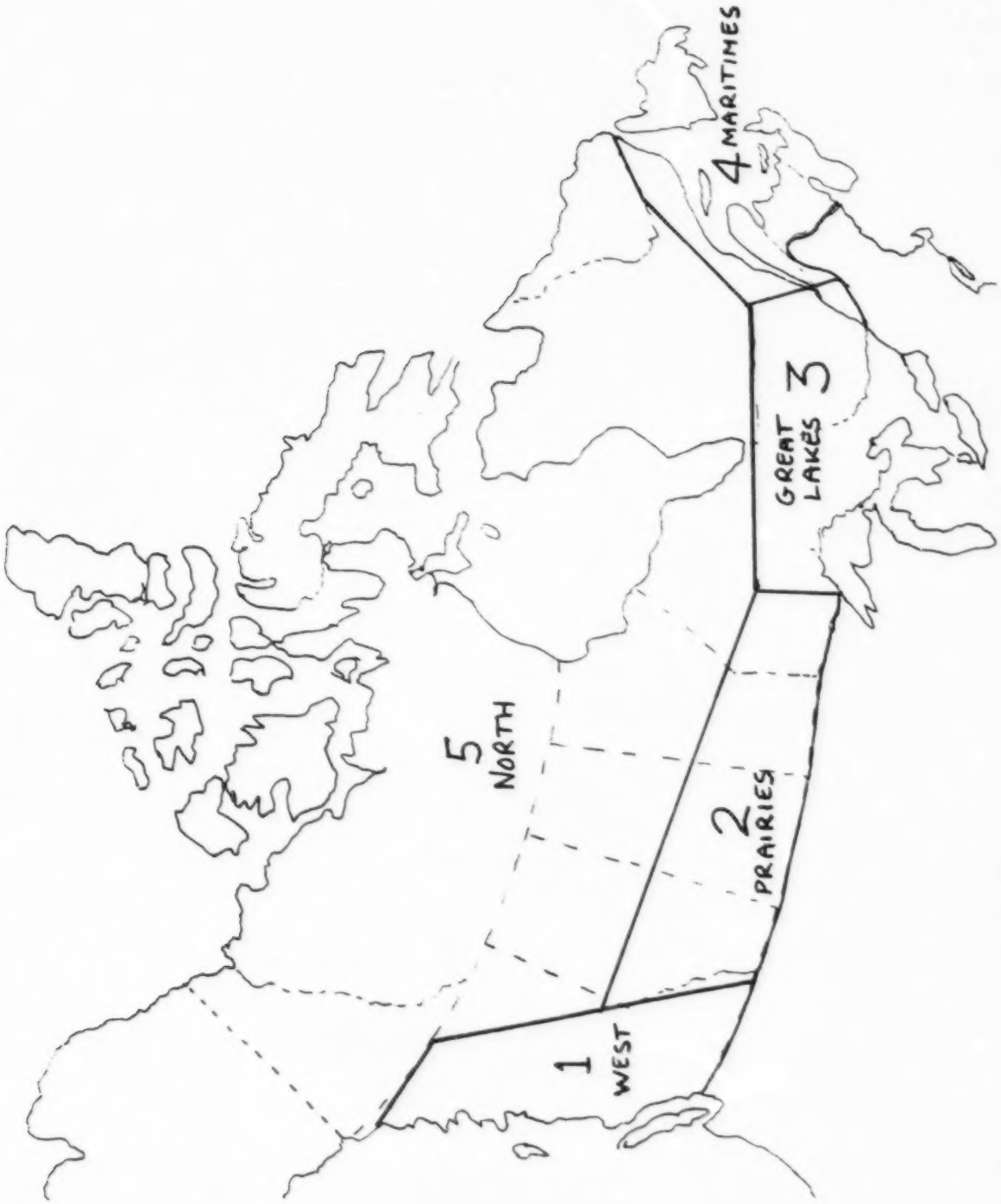
(d) The models and methods used should be totally open and available for use and comment by the public, universities, industry and other interested parties.

(e) When models become generally available, financial and human resources must be devoted to independent peer review and analysis, and to providing training and support from an accessible individual who is familiar enough with the model to answer questions about its structure. The strategy taken by US EPA Athens laboratory in providing support for models such as MINTEQ is an excellent example to follow. The promotion of models does not end with simply making available a diskette or tape. The model requires continuing validation, training, documentation and communication. Unfortunately this is likely to be expensive and many agencies have been reluctant to allocate these resources. It can be argued that if regulatory decisions are going to be based on models, there is an obligation on the part of the government decision maker to obtain this type of back-up. Only in this way will an unbiased credible system of chemical assessment be created under CEPA.

(f) When calculating exposures, it is better to estimate using both single number values and distributions of values. The lay public and the news media often attach too much significance to the numbers that are generated and focus on "worst case" situations. H&W should seek methods of communicating numbers in a more meaningful manner so that accuracy and significance are not misinterpreted and exposure not exaggerated.

A similar problem exists in describing tolerable or acceptable doses. Perhaps regulatory statements should express how closely a band or distribution of expected exposure matches a range of levels believed to be of concern (or no concern). In the case of existing chemicals, this could be backed up with a statement that continued reduction in toxic chemical exposure is being sought. The public is unlikely to accept our statement that exposure to dioxin at a level of Y ng/day is "acceptable". People are more likely to accept a claim that an exposure of 100 units/day is believed to cause no effects in the bulk population, especially if it is accompanied by an explanation that current exposures range from 5 to 25 and that we are seeking to identify the sources of the 5 to 25 and reduce them by a factor of 5 in the next few years. Often this reduction may require lifestyle changes, for example, in use of domestic chemicals. Those who want low exposure then have the knowledge to arrange their lives accordingly.

Figure 3.1
Suggested assessment regions in Canada.



4. Conclusions

A survey of existing environmental fate and human exposure models has been undertaken and the characteristics of the models documented.

No existing model is suitable for immediate adoption by the Department for assessing potential human exposure to new chemicals.

It is suggested that the Department develop a model or modelling capability applicable to Canadian conditions by modifying existing environmental fate and human exposure models, exploiting the best features of available models.

Adaption of the well-established fugacity approach for environmental fate assessment as is being done in Europe and Japan, would enable the Department to proceed immediately to build on it the exposure assessment phase of the process. A number of policy issues have been exposed and discussed briefly. These issues should be resolved at an early stage of model development. Of particular importance are:

1. the resources (person years and money) to be devoted to model development and maintenance,
2. relationships with the Department of Environment,
3. international implications, especially with the US and the EEC.

Because environmental fate and exposure modelling is in a state of evolution, it is desirable that the modelling approach taken be entirely open to public and industrial comment and peer review by the scientific community.

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Appendix

Table 3.2 – Summary of Quantitative Methods

Pathways	Equations	Definitions	Comments	Reference
PATHWAY TO ANIMALS (Section B.2)				
Ingestion of Contaminated Feed or Water				
	$C_T = (BF_f)(F)C_D$	C_T = conc. of chem. in tissue (µg/kg) BF_f = bioconcentration factor (fat basis) for organism of concern ((µg/kg fat)/(µg/kg of diet)) F = fat content of tissue (kg fat/kg tissue) C_D = concentration of pollutant in diet (or drinking water)(µg/kg)		
	Method 1 log BF_f = -1.476-0.495 log S = -3.457+0.500 log K_{ow} = -3.825+0.701 log K_{oc} = -3.839+0.869 log BCF_f = -2.842+0.674 log BCF_t	S = water solubility (ppm) K_{ow} = octanol-water partition coefficient K_{oc} = organic carbon water adsorption coefficient BCF_f = bioconcentration factor in fish in flowing water tests BCF_t = bioconcentration factor in fish in static water terrestrial systems.	Regression using 23 chemicals, mainly chlorinated herbicides and pesticides, and wide ranges of values for independent variables. Criticized by Garten and Trabalka (1983) for use of questionable data. Confidence limits covered nearly 4 orders of magnitude.	Kenaga (1980)
	Method 2 log K_{ow} ≤3.5; no appreciable bioaccumulation in fat; i.e. BF_f <0.3 log S >4; No appreciable bioaccumulation in fat; i.e., BF_f <0.03	As above	Screening levels only. False positive/false negative error rate of 25% with 68 chemicals. Not applicable to chemicals that can covalently bond or bind to proteins rather than fat.	Garten and Trabalka (1983)
Inhalation of Pollutants in Air				
	No Available Method			
Dermal Absorption				
	$F_s = K_s \Delta C$	F_s = flux or permeation rate through skin (mg/cm^2-hr) K_s = permeability constant (l/cm^2-hr) ΔC = concentration difference across skin (mg/l)	Fick's Law	Brown et al (1984)
	$K_{si} = K_{sj} (MW_j/MW_i)^{1/2}$	K_{si} = permeability constant of chemical i (l/cm^2-hr) K_{sj} = permeability constant of chemical j (l/cm^2-hr) MW_i = molecular weight of chemical i MW_j = molecular weight of chemical j		U.S. EPA (1985)

Summary of Quantitative Methods (cont'd)

Pathways	Equations	Definitions	Comments	Reference
PATHWAYS TO FISH/SHELLFISH (Section B.3)				
	$C_{ao} = (BCF)C_w$	BCF = bioconcentration factor in fish (µg/kg / µg/l) C_{ao} = concentration of pollutant in aquatic organism at equilbrium (µg/kg) C_w = concentration of pollutant in water (µg/l)		
	Method 1 log BCF= 0.76 log K_{ow}-0.23 = 2.791-0.564 log S = 1.119 log K_{oc}-1.579	Kow = octanol-water partition coefficient S = water solubility (ppm) K_{oc} = soil (or sediment) adsorption coefficient	Regression with 84 chemicals and K_{ow} between 7.9 to 8.1 × 10^6. Regression with 46 chemicals and S between 0.001 and 50,000 ppm. Regression with 13 chemicals and K_{oc} 1 to 1.2 × 106. Wide classes of chemicals represented by equations, but only a few fish species.	Bysshe (1982)
	Method 2 BCF = 0.048 K_{ow}	As above	Used by EPA's TOX-SCREEN, screening level program.	Mackay (1982)
PATHWAYS TO CROPS (Section B.4)				
Uptake from Air				
	Method 1 $C_p = C_a RT/H$	C_p = concentration of pollutant in plant (µg/ml) C_a = concentration of pollutant in air (µg/ml) H = Henry's Law Constant (m^3 atm/mol) R = Gas Constant (8.2 x 10^{-5} m^3 atm/mol °K) T = Temperature (°K)	Theoretical, not tested with empirical experimental data.	
	Method 2 $C_p = \frac{r}{Y_v \lambda_{ei}} [1-(1-e^{-\lambda_{ei} t_e})/(\lambda_{ei} t_e)]$ x (deposition rate)	r = empirically determined initial reception fraction Y_v = vegetative productivity (g/m^2) λ_{ei} = empirical weathering constant (day^{-1}) t_e = crop growth period before harvest or grazing (days) deposition rate (g/m^2-day)	Equation derived from interception of radionuclides. A number of empirical values required which are unknown for organic chemicals.	Chamberlain (1970)

Summary of Quantitative Methods (cont'd)

Pathways	Equations	Definitions	Comments	Reference
Root Uptake				
	Method 1 $RCF = C_R/C_{ex}$	RCF = root concentration factor C_R = concentration in roots (μg/ml) C_{ex} = concentration in external solution (μg/ml)		Briggs et al (1982)
	$TSCF = C_w/C_{ex}$	TSCF = transpiration stream concentration factor C_w = concentration in transpiration stream (μg/ml) C_{ex} = concentration in external solution (μg/ml)		Briggs et al (1982)
	$\log (RCF-0.82) = 0.77 \log K_{ow}-1.52$ $TSCF = 0.784 \exp-((\log K_{ow}-1.78)^2/2.44))$ $RCF = 0.82$ (for polar species)	K_{ow} = octanol-water partition coefficient	Regression equations for 18 compounds (non-ionic 0-methyl-carbamoyloximes and substituted phenylureas) in barley shoots grown in nutrient solutions. Root physiology or rapid metabolism in roots may result in lower TSCF values than predicted.	Briggs et al (1982)
	Method 2 $RCF_s = C_R/C_s$ $TSCF_s = C_w/C_s$ $\log (RCF_s K_{oc}(OC)-0.82) = 0.77 \log K_{ow}-1.52$ $TSCF_s K_{oc}(OC) = 0.784 \exp-((\log K_{ow} - 1.78)^2/2.44))$ $RCF_s K_{oc}(OC) = 0.82$ (for polar species)	C_s = total concentration in soil ($\mu g/cm^3$) Other definitions as above K_{oc} = soil adsorption coefficient OC = fractional organic carbon (g/g) Other definitions as above	As above	Derived from Briggs et al (1982)
	Method 3 $C_{pl} = BC_{pl} \times C_o$ $K_d = K_{oc}$ (%OC) $\ln K_d = A+B \ln (BC_{pl})$ or $\ln (K_{oc}(\%OC)) = A+B\ln(BC_{pl})$	C_{pl} = mature plant parts concentration (μg/g dry weight) BC_{pl} = bioconcentration factor in mature plant parts C_o = soil concentration (μg/g dry weight) K_d = soil-water partition coefficient K_{oc} = soil adsorption coefficient %OC= percent organic carbon A and B are empirically derived constants	Used by EPA's TOXSCREEN, screening level program. Values of A and B used in TOXSCREEN are 3.02 and -0.85 respectively based on literature review o 21 elements	USEPA (1984b)

Summary of Quantitative Methods (cont'd)

Pathways	Equations	Definitions	Comments	Reference
PATHWAYS TO FOOD-POST-HARVEST STAGES (Section B.5)				
Food in Contact with Air, Water or Liquid				
	DIFFUSION: $F = -D(dC/dx)$	F = pollutant mass flux along direction × (μg/cm²-sec) D = diffusion coefficient of pollutant in food (cm²/sec) C = concentration of pollutant in medium (μg/ml) dC/dx = concentration gradient in direction × (μg/ml-cm)	Fick's law	
	From Air to Food Air $F_1 = D_{fa}^*(C_a - C_{fa})/r$	F_1 = pollutant mass flux across food surface (μg/cm²-sec) D_{fa}^* = apparent diffusion coefficient of pollutant in food air (cm²/sec) C_a = concentration of pollutant in air (μg/ml) C_{fa} = concentration of pollutant in food air (μg/ml) r = approx. radius of food particle (cm)	Many independent variables may have to be estimated. Additional equations for estimation of these parameters are shown in Appendix B or references provided.	
	$D_{fa}^* = D_a(n_{air}^{10/3}/n_f^2)$	D_a = diffusion coefficient of pollutant in air (cm²/sec) n_{air} = food-air filled porosity (ml/ml) n_f = food (total) porosity (ml/ml) m = food water content (ml/ml)		
	$n_{air} = n_f - m$			
	$\bar{F}_1 = F_1/2$ for $C_{fa} = 0, t = 0$ sec	$\bar{F}_1$ = average pollutant mass flux across surface (μg/cm²-sec)	Estimates average concentration in food. Concentration varies spatially and with exposure time. Does not consider deposition of particulates.	
	$C_t = C_i + (\bar{F}_1 At)/M$	C_t = concentration of pollutant in food after time t (mg/kg) C_i = initial pollutant concentration in food (μg/kg) t = time (sec) M = mass of food piece (kg) A = surface area of food piece (cm²)		
	From External Liquid to Food Liquid $F_2 = D_{fm}^*(C_{el} - C_{fm})/r$	F_2 = pollutant mass flux across food surface (μg/cm²-sec) D_{fm}^* = apparent diffusion coefficient in food moisture (cm²/sec) C_{el} = concentration of pollutant in external liquid (μg/ml) C_{fm} = concentration of pollutant in food moisture (μg/ml) r = approx. radius of food particle (cm)	Many independent variables may have to be estimated. Estimation methods provided in Appendix B or references provided.	

Summary of Quantitative Methods (cont'd)

Pathways	Equations	Definitions	Comments	Reference
	Similar equations as diffusion from air to food air	Similar definitions as diffusion from air to food air	Estimates average concentration in food. Concentration varies spatially and with exposure time.	
	PARTITIONING:			
	Moisture-Solid Partitioning $S = x/M = KC_{el}1/n$	S = adsorbed concentration of contaminant on food particles (μg/g food) x = adsorbed pollutant mass on/in food (μg) M = mass of food (g) K = adsorption (partitioning) coefficient (μg/g)/(μg/ml) C_{el} = dissolved concentration of pollutant in external liquid (μg/ml) n = Freundlich isotherm parameter K_{ow} = octanol-water partition coefficient	Equations adapted from similar equations derived for organic soils and assumed valid for food. Assumes equilibrium.	
	$K = K_{ow}$ (lipid)/100			
	Moisture-Air Partitioning $C_{fa} = C_{fm}$ H/RT	C_{fa} = concentration in food-air (μg/ml) C_{fm} = concentration in food-moisure (μg/ml) H = Henry's law Constant (m^3 atm/mol °K) R = gas constant (8.2×10^{-5}) m^3 atm/mol °K) T = temperature (°K)	Derived from Henry's law applicable to dilute solutions. Theoretical. Food solution is usually not dilute.	
Food in Contact with Surfaces	$M_t = 2C_{op}(D_p t/\pi)^{1/2}$	M_t = amount migrated at time t (g/cm^2) C_{op} = initial chemical concentration in surface (g/cm^3) D_p = effective diffusion coefficient through surface (cm^2/sec) t = time of contact of food with surface (sec)	For porous surfaces, e.g., soil, gives maximum amount of chemical that could migrate out.	Schwope et al. (1984)
	$D_p = D_a(n_{air}10/3/n_s2)$	D_a = diffusion coefficient of pollutant in air (cm^2/sec) n_{air} = surface air-filled porosity (ml/ml) n_s = surface total porosity (ml/ml)		
	$C_f = 2C_{op}(D_p t/\pi)^{1/2} A_f/V_f$	C_f = average concentration of chemical in food (g/cm^3) A_f = surface area of food in contact with surface (cm^2) V_f = volume of food (cm^3)	Gives maximum average concentration in food. Concentrations would vary spatially.	

Summary of Quantitative Methods (cont'd)

Pathways	Equations	Definitions	Comments	Reference
	Max. Conc. is limited by: $K = K_{ow}$ (% lipid)/100	K = adsorption (partitioning) coefficient (μg/g)/(μg/ml) K_{ow} = octanol-water partition coefficient	Assumes equilibrium.	
Additives	$C_f = C_i + \frac{C_a M_a}{M_f + M_a}$	C_f = final concentration of the pollutant in food (μg/kg) Ci = initial concentration of pollutant in food (μg/kg) C_a = concentration of pollutant in additive (μg/kg) M_a = mass of substance added (kg) M_f = mass of food to which substance was added (kg)	Concentration of substance in additive and mass of additive needs to be known.	
CHEMICAL LOSES (Section B.6)				
	Similar to the equations for pathways to food-post-harvest stages.			

References to Appendix

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